

Burch  
10/6 93315

Page 1

=> dis his

(FILE 'HOME' ENTERED AT 16:08:17 ON 13 DEC 2005)

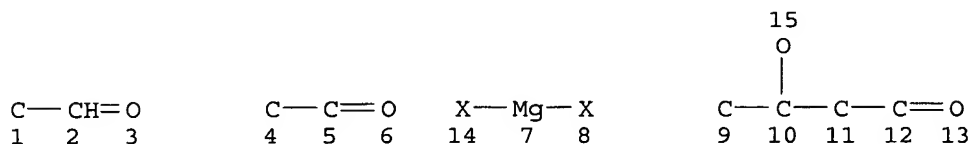
FILE 'REGISTRY' ENTERED AT 16:08:21 ON 13 DEC 2005

FILE 'CASREACT' ENTERED AT 16:08:24 ON 13 DEC 2005

L1 STR  
L2 6 S L1  
L3 118 S L1 FUL  
L4 STR  
L5 77 SEARCH L4 SUB=L3 FUL  
L6 41 S L3 NOT L5

=> d l6 que stat

L1 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE

L3 118 SEA FILE=CASREACT SSS FUL L1 ( 1302 REACTIONS)

L4 STR

Li 1

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 1

STEREO ATTRIBUTES: NONE

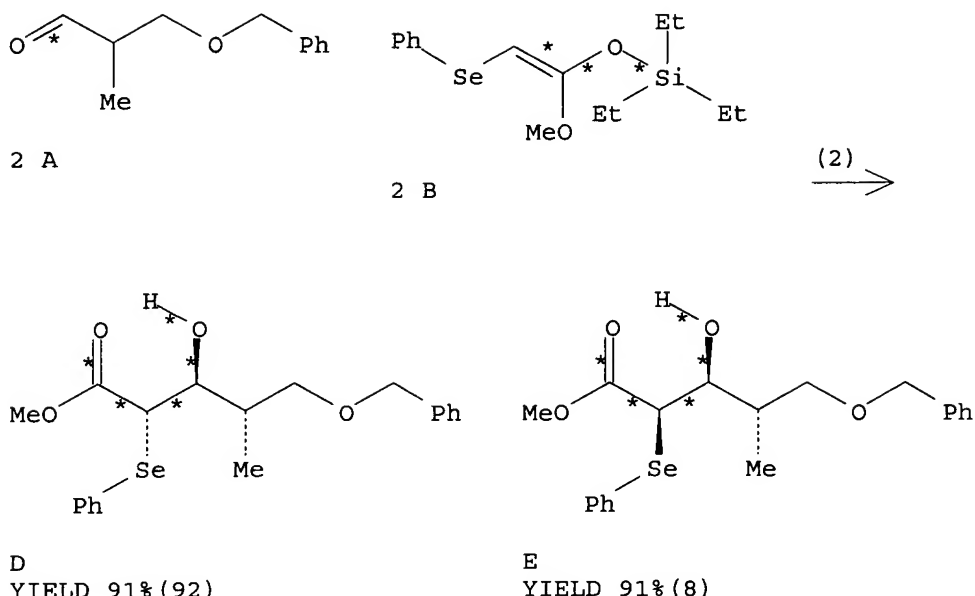
L5 77 SEA FILE=CASREACT SUB=L3 SSS FUL L4 ( 1060 REACTIONS)

L6 41 SEA FILE=CASREACT ABB=ON PLU=ON L3 NOT L5

=> d 1-41 fhit bib abs

L6 ANSWER 1 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(2) OF 112 2 A + 2 B ==> D + E...



RX(2) RCT A 73814-73-0, B 367264-15-1

STAGE(1)

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 10 minutes, -78 deg C

STAGE(2)

RGT H 29858-07-9 MgBr<sub>2</sub>-Et<sub>2</sub>O  
CON -78 deg C

PRO D 367264-27-5, E 367264-28-6

NTE stereoselective, the yield and stereoselectivity depend on the reaction conditions and on the Lewis acid used

AN 142:240074 CASREACT

TI Synthesis of Tertiary and Quaternary Stereogenic Centers: A Diastereoselective Tandem Reaction Sequence Combining Mukaiyama and Free Radical-Based Allylation

AU Cardinal-David, Benoit; Guerin, Brigitte; Guindon, Yvan

CS Bio-organic Chemistry Laboratory, Institut de recherches cliniques de Montreal (IRCM), Montreal, QC, H2W 1R7, Can.

SO Journal of Organic Chemistry (2005), 70(3), 776-784  
CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

LA English

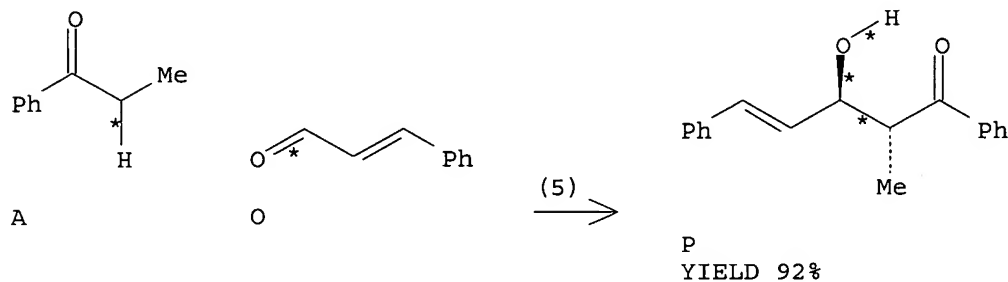
AB A strategy employing a Mukaiyama reaction in tandem with a free radical-based allyl transfer reaction for the elaboration of functionalized tertiary and quaternary centers is reported. The appropriate choice of alc.-protecting group on the starting  $\alpha$ -methyl- $\beta$ -hydroxyaldehyde ROCH<sub>2</sub>CHMeCHO (R = Me<sub>3</sub>CSiMe<sub>2</sub>, PhCH<sub>2</sub>) and the nature of the Lewis acid used in the Mukaiyama reaction provided access to 3,4-anti and 3,4-syn aldolization products, precursors of the free-radical allylation reaction. After migration or exchange of the Lewis acid, the allyl transfer reaction with allyltributylstannane is then performed by taking advantage of the endocyclic effect, leading to the

2,3-anti relative stereochem. Importantly,  $^{13}\text{C}$  NMR studies of the chelated intermediates are also reported and provide addnl. support for the endocyclic effect. In some cases, the remarkable reactivity of the aluminum-based Lewis acids allowed the use of allyltrimethylsilane, an interesting reagent from an ecol. standpoint. The isolation of a key intermediate is also indicative of an atom transfer mechanism when the silicon-based reagent is employed.

RE.CNT 85 THERE ARE 85 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(5) OF 16 A + O ==> P



RX(5) RCT A 93-55-0, O 104-55-2

STAGE(1)

RGT D 10377-58-9 MgI<sub>2</sub>, E 110-89-4 Piperidine  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 2 hours, room temperature

STAGE(2)

RGT F 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

PRO P 187848-84-6

NTE stereoselective, anti:syn 88:12

AN 142:113673 CASREACT

TI Anti-selective and regioselective aldol addition of ketones with aldehydes using MgI<sub>2</sub> as promoter

AU Wei, Han-Xun; Jasoni, Richard L.; Shao, Huawu; Hu, Jiali; Pare, Paul W.

CS Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX, 79409, USA

SO Tetrahedron (2004), 60(51), 11829-11835

CODEN: TETRAB; ISSN: 0040-4020

PB Elsevier B.V.

DT Journal

LA English

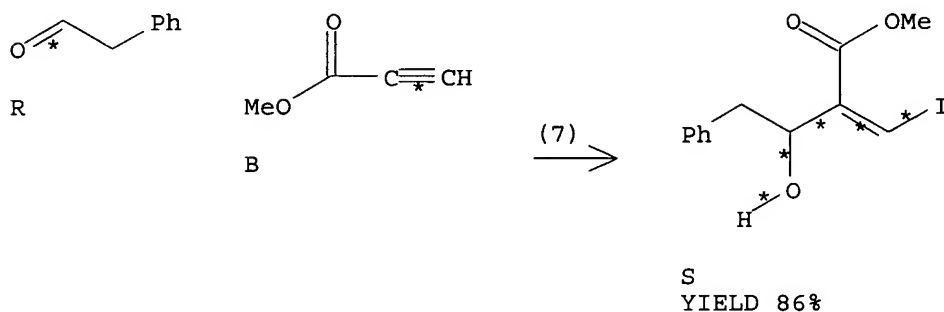
AB The first example of a direct aldehyde-ketone coupling using the secondary amine piperidine as base in the presence of MgI<sub>2</sub> to generate high selectivity of anti-aldol products from unmodified Et ketones in high yield is reported. The coupling reactions were carried out in a one-pot reaction by mixing four reaction components at room temperature. In the case of unsym. ketones, addition was made to the less hindered  $\alpha$ -side.

RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(7) OF 10 R + B ==&gt; S



RX(7) RCT R 122-78-1

STAGE(1)

RGT D 10377-58-9 MgI2

SOL 75-09-2 CH2Cl2

CON 20 minutes, room temperature

STAGE(2)

RCT B 922-67-8

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) 1 hour, room temperature

STAGE(3)

RGT E 7647-01-0 HCl

SOL 7732-18-5 Water

CON room temperature

PRO S 643761-27-7

NTE stereoselective, Baylis-Hillman reaction

AN 142:37987 CASREACT

TI Synthesis of substituted  $\alpha$ -(hydroxymethyl)- $\beta$ -iodoacrylates via  
MgI2-promoted stereoselective aldol coupling

AU Wei, Han-Xun; Hu, Jiali; Jasoni, Richard L.; Li, Guigen; Pare, Paul W.

CS Department of Chemistry and Biochemistry, Texas Tech University, Lubbock,  
TX, 79409, USA

SO Helvetica Chimica Acta (2004), 87(9), 2359-2363

CODEN: HCACAV; ISSN: 0018-019X

PB Verlag Helvetica Chimica Acta

DT Journal

LA English

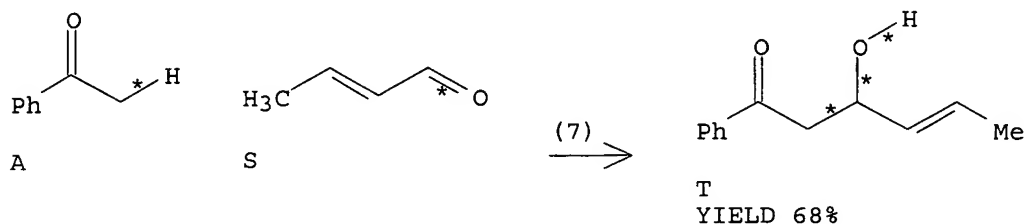
AB The efficient and highly stereoselective syntheses of a variety of  
(Z)-configured, substituted  $\alpha$ -(hydroxymethyl)- $\beta$ -iodo-acrylates  
RCH(OH)C(CO2Me):CHI (R = Ph, n-Bu, 2-naphthyl, etc.) from Me prop-2-ynoate  
and various aldehydes RCHO was achieved. The synthetic protocol involves  
a simple one-pot coupling reaction under mild conditions, promoted by  
MgI2, which serves both as a Lewis acid and iodine source for a  
Baylis-Hillman-type reaction. All adducts were generated in  
good-to-excellent yields, the (Z)-isomers being formed in high selectivity

(> 98%). The conversion of Me prop-2-ynoate into an active ' $\beta$ -iodo allenolate' intermediate, which then nucleophilically attacks an aldehyde, is proposed as a plausible reaction mechanism.

RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(7) OF 12 A + S ==> T



RX(7) RCT A 98-86-2, S 4170-30-3

STAGE(1)

RGT D 10377-58-9 MgI<sub>2</sub>, E 7087-68-5 EtN(Pr-i)<sub>2</sub>  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
CON 30 minutes, room temperature

STAGE(2)

RGT F 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

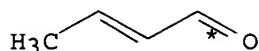
PRO T 112586-63-7

AN 142:37977 CASREACT  
TI Versatile one-step one-pot direct aldol condensation promoted by MgI<sub>2</sub>  
AU Wei, Han-Xun; Li, Kunyu; Zhang, Qian; Jasoni, Richard L.; Hu, Jiali; Pare, Paul W.  
CS Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX, 79409, USA  
SO Helvetica Chimica Acta (2004), 87(9), 2354-2358  
CODEN: HCACAV; ISSN: 0018-019X  
PB Verlag Helvetica Chimica Acta  
DT Journal  
LA English  
AB A true one-step one-pot aldol-reaction procedure has been developed for the synthesis of  $\beta$ -hydroxy ketones and esters from RCOMe [R = Ph, 4-FC<sub>6</sub>H<sub>4</sub>, 4-MeOC<sub>6</sub>H<sub>4</sub>, (1,1'-biphenyl)-4-yl, MeO, EtO, PhO] and R<sub>1</sub>CHO (R<sub>1</sub> = Ph, 4-MeOC<sub>6</sub>H<sub>4</sub>, 4-FC<sub>6</sub>H<sub>4</sub>, MeCH:CH, Et). The reaction can be run at room temperature by simply mixing four components in CH<sub>2</sub>Cl<sub>2</sub>, with medium-to-high yields of aldol products obtained after regular workup. Mechanistically, the process probably proceeds via Mg-enolate formation of the ketone or ester component, followed by addition to the electrophilic aldehyde.

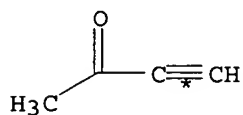
RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

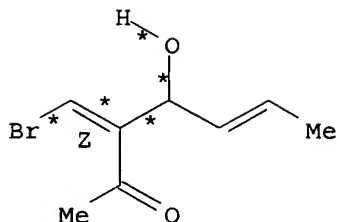
RX(6) OF 10      2 U + 2 B ==> V + W



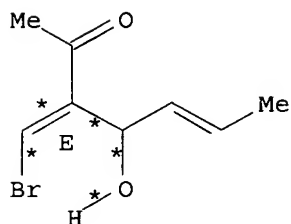
2 U .



2 B



V  
YIELD 84%(82)



W  
YIELD 84%(18)

RX(6)      RCT   U 4170-30-3, B 1423-60-5

STAGE(1)

RGT   E 7789-48-2 MgBr2  
SOL   75-09-2 CH2Cl2  
CON   5 hours, room temperature

STAGE(2)

RGT   F 144-55-8 NaHCO3  
SOL   7732-18-5 Water  
CON   room temperature

PRO   V 797751-04-3, W 797751-11-2

NTE   stereoselective, Bayliss-Hillman reaction

AN   142:6219   CASREACT

TI   Z/E Stereoselective synthesis of β-bromo Baylis-Hillman ketones using MgBr2 as promoter via a one-pot three-component reaction

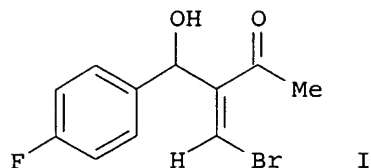
AU   Wei, Han-Xun; Jasoni, Richard L.; Hu, Jiali; Li, Guigen; Pare, Paul W.

CS   Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX, 79409, USA

SO   Tetrahedron (2004), 60(45), 10233-10237

CODEN: TETRAB; ISSN: 0040-4020

PB Elsevier B.V.  
 DT Journal  
 LA English  
 GI

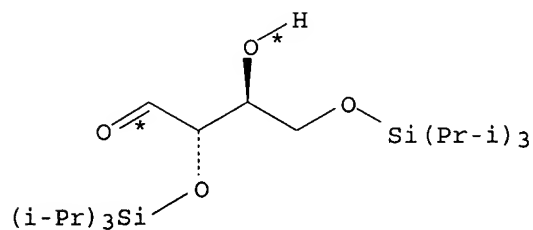


AB The stereoselective synthesis of (Z)- $\beta$ -bromo Baylis-Hillman ketones, e.g., I, has been achieved using a one-pot three-component reaction. The system used  $\text{MgBr}_2$  as both the Lewis acidic promoter and the bromine source for the Michael-type addition to  $\alpha,\beta$ -acetylenic ketones to form an active  $\beta$ -bromo allenolate intermediate, which in turn attacked various aldehydes to afford  $\beta$ -bromo Baylis-Hillman adducts in good yields and Z-selectivity.

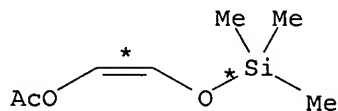
RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 6 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(13) OF 114 ...2 AN + 2 C ==> AO + AP...

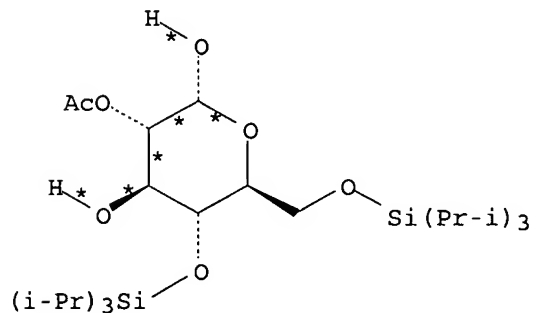


2 AN

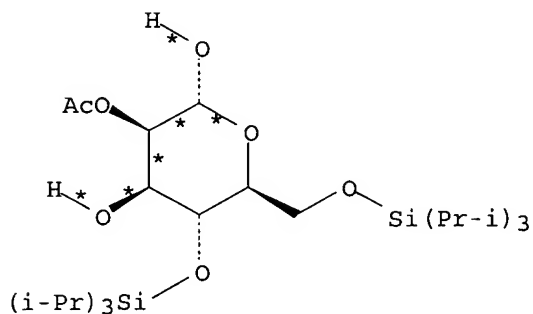


2 C

(13)  $\longrightarrow$



AO  
 YIELD 74%



AP  
YIELD 5%

RX(13) RCT AN 700367-77-7

STAGE(1)

RGT AQ 29858-07-9 MgBr2-Et2O  
SOL 60-29-7 Et2O  
CON SUBSTAGE(1) room temperature -> -20 deg C  
SUBSTAGE(2) 30 minutes, -20 deg C

STAGE(2)

RCT C 792931-85-2  
CON SUBSTAGE(1) 2 hours, -20 deg C  
SUBSTAGE(2) 4 hours, -20 deg C -> 4 deg C  
SUBSTAGE(3) 24 hours, 4 deg C

STAGE(3)

RGT AF 12125-02-9 NH4Cl  
SOL 7732-18-5 Water  
CON 4 deg C, acidify

STAGE(4)

RGT AR 110-54-3 Hexane  
SOL 7732-18-5 Water, 109-99-9 THF  
CON 30 minutes, 0 deg C

STAGE(5)


RGT M 144-55-8 NaHCO3  
SOL 7732-18-5 Water  
CON basify

PRO AO 792931-86-3, AP 792931-87-4  
NTE stereoselective

AN 141:411171 CASREACT  
TI Two-Step Synthesis of Carbohydrates by Selective Aldol Reactions  
AU Northrup, Alan B.; MacMillan, David W. C.  
CS Department of Chemistry, California Institute of Technology, Pasadena, CA, 91125, USA  
SO Science (Washington, DC, United States) (2004), 305(5691), 1752-1755  
CODEN: SCIEAS; ISSN: 0036-8075  
PB American Association for the Advancement of Science  
DT Journal  
LA English



L6 ANSWER 7 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

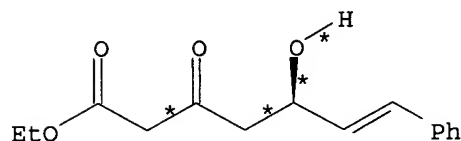


I

J

Q

2  
STEPS  
→



RX (3) RCT I 101979-45-7

```
STAGE(1)
  RGT  L 7550-45-0 TiCl4
  SOL  75-09-2 CH2Cl2
  CON  SUBSTAGE(1) room temperature -> -78 deg C
        SUBSTAGE(2) -78 deg C -> -40 deg C
        SUBSTAGE(3) 10 minutes, -40 deg C
        SUBSTAGE(4) -40 deg C -> -78 deg C
```

```

STAGE(2)
  RGT  M 7087-68-5 EtN(Pr-i)2
  CON  SUBSTAGE(1) -78 deg C -> -40 deg C
        SUBSTAGE(2) 2 hours, -40 deg C
        SUBSTAGE(3) -40 deg C -> -78 deg C

```

STAGE(3)

RCT J 14371-10-9  
CON 1 hour, -78 deg C

STAGE(4)

RGT N 12125-02-9 NH4Cl  
SOL 7732-18-5 Water

PRO K 101979-49-1  
NTE stereoselective, aldol reaction

RX(4) RCT K 101979-49-1, Q 6148-64-7

STAGE(1)

RGT R 7786-30-3 MgCl2  
SOL 109-99-9 THF  
CON 30 minutes, room temperature

STAGE(2)

RGT S 288-32-4 1H-Imidazole  
CON overnight, room temperature

PRO A 735287-46-4

AN 141:174012 CASREACT

TI Versatile Asymmetric Synthesis of the Kavalactones: First Synthesis of (+)-Kavain

AU Smith, Thomas E.; Djang, Mabel; Velander, Alan J.; Downey, C. Wade; Carroll, Kathleen A.; Van Alphen, Sophie

CS Department of Chemistry, Williams College, Williamstown, MA, 01267, USA

SO Organic Letters (2004), 6(14), 2317-2320

CODEN: ORLEF7; ISSN: 1523-7060

PB American Chemical Society

DT Journal

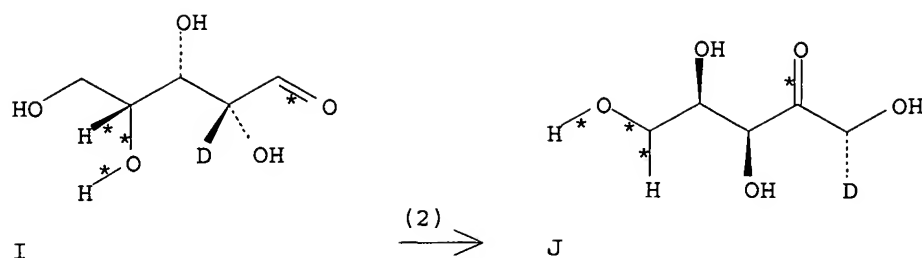
LA English

AB Three asym. pathways to the kavalactones were developed. The first method is chiral auxiliary-based and utilizes aldol reactions of N-acetyl thiazolidinethiones followed by a malonate displacement/decarboxylation reaction. The second approach uses the asym. catalytic Mukaiyama addns. of dienolate nucleophile equivalent developed by Carreira and Sato. Finally, tin-substituted intermediates, prepared by either of these routes, can serve as advanced general precursors of kavalactone derivs. via Pd(0)-catalyzed Stille couplings with aryl halides.

RE.CNT 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 8 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(2) OF 5 I ==> J



RX(2) RCT I 288846-91-3  
 RGT C 56-65-5 Adenosine 5'-(tetrahydrogen triphosphate), D  
 7786-30-3 MgCl<sub>2</sub>, E 590-54-5 Acetic acid,  
 monoanhydride with phosphoric acid  
 PRO J 721449-15-6  
 CAT 9023-82-9 Isomerase, xylose, 9030-58-4 Kinase (phosphorylating),  
 xylulo-, 9027-42-3 Kinase (phosphorylating), acetate  
 SOL 7732-18-5 Water  
 CON 3 hours, 25 deg C, pH 7  
 NTE biotransformation, enzymic, maleate buffered soln.,  
 regioselective

AN 141:119183 CASREACT

TI Evolution of Enzymatic Activities in the Orotidine 5'-Monophosphate  
 Decarboxylase Suprafamily: Mechanistic Evidence for a Proton Relay System  
 in the Active Site of 3-Keto-L-gulonate 6-Phosphate Decarboxylase

AU Yew, Wen Shan; Wise, Eric L.; Rayment, Ivan; Gerlt, John A.

CS Departments of Biochemistry and Chemistry, University of Illinois, Urbana,  
 IL, 61801, USA

SO Biochemistry (2004), 43(21), 6427-6437

CODEN: BICHAW; ISSN: 0006-2960

PB American Chemical Society

DT Journal

LA English

AB 3-Keto-L-gulonate 6-phosphate decarboxylase (KGPDC) and orotidine  
 5'-monophosphate decarboxylase (OMPDC) are homologous enzymes that share  
 the (β/α)<sub>8</sub>-fold but catalyze mechanistically distinct reactions  
 [Wise, E., Yew, W. S., Babbitt, P. C., Gerlt, J. A., and Rayment, I.  
 (2002) Biochem. 41, 3861-3869]. KGPDC catalyzes the Mg<sup>2+</sup>-dependent  
 decarboxylation of 3-keto-L-gulonate 6-phosphate, an intermediate in the  
 catabolic pathway of L-ascorbate utilization by Escherichia coli K-12  
 [Yew, W. S., and Gerlt, J. A. (2002) J. Bacteriol. 184, 302-306]. OMPDC  
 catalyzes a metal ion-independent reaction that likely proceeds without a  
 vinyl anion intermediate [Appleby, T. C., Kinsland, C., Begley, T., and  
 Ealick, S. E. (2000) Proc. Natl. Acad. Sci. U.S.A. 97, 2005-2010],  
 although the mechanistic details are uncertain. An active site Lys  
 located at the end of the third β-strand in OMPDC has been proposed  
 to be the general acid that delivers a solvent-derived proton to the UMP  
 product; the active site of KGPDC contains a homologous Lys residue  
 (Lys64). Herein, we report investigations of the KGPDC-catalyzed reaction  
 that are consistent with a mechanism involving a Mg<sup>2+</sup>-stabilized  
 cis-enediolate intermediate [Wise, E. L., Yew, W. S., Gerlt, J. A., and  
 Rayment, I. (2003) Biochem. 42, 12133-12142] and implicate waters proximal  
 to His136 and Arg139, both located at the end of the sixth β-strand,  
 as the general acids that deliver a solvent-derived proton to the  
 intermediate to form the L-xylulose 5-phosphate product. On the basis of  
 our mechanistic investigations, Lys64 stabilizes the cis-enediolate  
 intermediate by forming hydrogen bonds to both O1 and O2 of the



enzymes available com., Tris-HCl buffered soln., stereoselective

AN 141:5851 CASREACT

TI A facile enzymatic synthesis of isotopically labeled 2-methyl-D-erythritol 2,4-cyclodiphosphate by spinach chloroplast stroma

AU Gao, Wenyun; Raschke, Maja; Alpermann, Henriette; Zenk, Meinhard H.

CS Biozentrum, Martin Luther-Universitaet Halle-Wittenberg, Halle/Saale, D-06120, Germany

SO Helvetica Chimica Acta (2003), 86(11), 3568-3577  
CODEN: HCACAV; ISSN: 0018-019X

PB Verlag Helvetica Chimica Acta

DT Journal

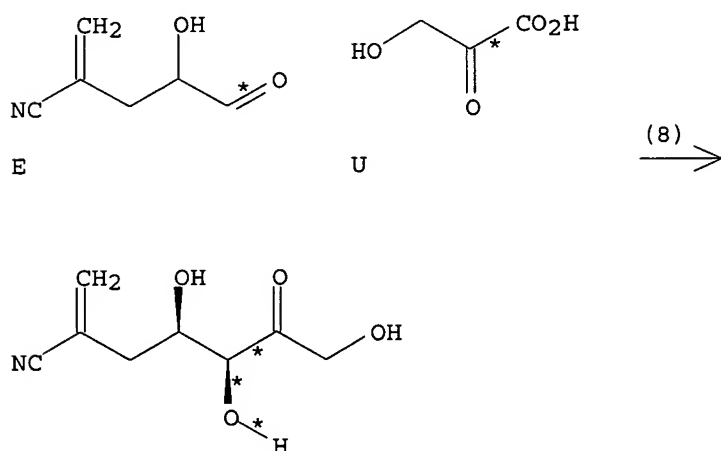
LA English

AB For the investigation of the ultimate and penultimate steps of the deoxyxylulose phosphate pathway in plants and microorganisms, and to solve intracellular transport problems, we have developed a facile enzymic preparation of 2-methyl-D-erythritol 2,4-cyclodiphosphate in highly radioactive form. Use has been made of spinach chloroplast stroma, as well as the stroma of *Capsicum annuum* and *Narcissus pseudonarcissus* chromoplasts, which were shown to transform differently labeled 1-deoxy-D-xylulose 5-phosphate quant. into that cyclic diphosphate in the presence of cofactors. This method can also be exploited to synthesize milligram quantities of <sup>13</sup>C-labeled cyclic diphosphate. It is shown that recombinant *Escherichia coli* deoxyxylulose phosphate synthase is catalytically active and can be used to synthesize the labeled starting material for further enzymic work, as well as for feeding of intact plants. The pH and temperature stability of the deoxyxylulose 5-phosphate and the cyclic diphosphate have been determined. Uniformly <sup>13</sup>C- or <sup>14</sup>C-labeled pyruvate, and uniformly <sup>13</sup>C- or <sup>14</sup>C-labeled D-glyceraldehyde 3-phosphate were synthesized in almost quant. yields from uniformly <sup>13</sup>C- or <sup>14</sup>C-labeled D-glucose en route to deoxyxylulose 5-phosphate.

RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 10 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(8) OF 46 ...E + U ==> V...



V  
YIELD 73%

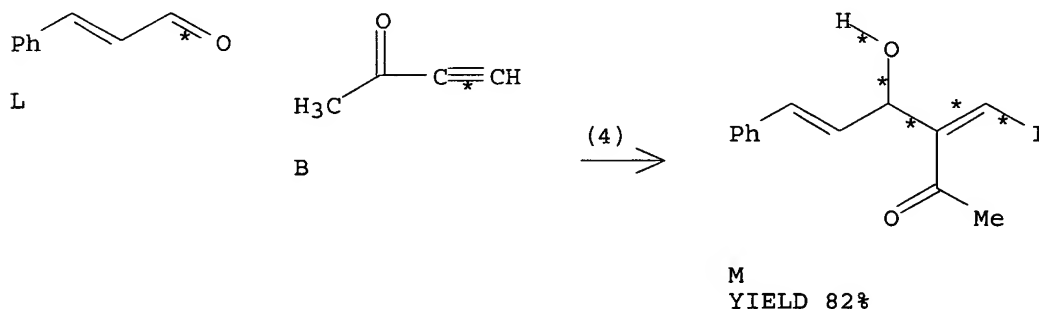
RX(8) RCT E 356788-23-3, U 1113-60-6  
 RGT W 7786-30-3 MgCl<sub>2</sub>, X 917-23-7 Tetraphenylporphine  
 PRO V 681826-38-0  
 SOL 7732-18-5 Water  
 CON 14 hours, room temperature  
 NTE biotransformation, enzymic, stereoselective, in the dark,  
 transketolase from *S. cerevisiae* used

AN 140:357578 CASREACT  
 TI Transketolase and fructose-1,6-bis-phosphate aldolase, complementary tools  
 for access to new ulosonic acid analogs  
 AU Crestia, Dominique; Demuynck, Colette; Bolte, Jean  
 CS Laboratoire de Synthèse et Etude de Systèmes à Interêt Biologique,  
 Université Blaise Pascal, UMR 6504 du CNRS, Aubière, 63177, Fr.  
 SO Tetrahedron (2004), 60(10), 2417-2425  
 CODEN: TETRAB; ISSN: 0040-4020  
 PB Elsevier Science B.V.  
 DT Journal  
 LA English  
 AB A new approach to the synthesis of ulosonic acids KDO and DAH is  
 described. The key step is the C5-C6 bond formation catalyzed by  
 fructose-1,6-bis-phosphate aldolase (for KDO) or transketolase (for DAH)  
 using substituted acrylonitrile  $\alpha$ -hydroxy-aldehyde. All asym.  
 carbon configurations are determined in an enzymic step by the means of  
 dehydrogenase or lipase. This strategy, using a non-metabolism pathway,  
 allows access to novel precursors of KDO, DAH and analogs.

RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 11 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(4) OF 10 L + B ==> M



RX(4) RCT L 14371-10-9

STAGE(1)

RGT D 10377-58-9 MgI<sub>2</sub>  
 SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
 CON SUBSTAGE(1) 20 minutes, room temperature  
 SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)

RCT B 1423-60-5  
 CON 1 hour, 0 deg C

STAGE(3)

RGT E 144-55-8 NaHCO3  
SOL 7732-18-5 Water

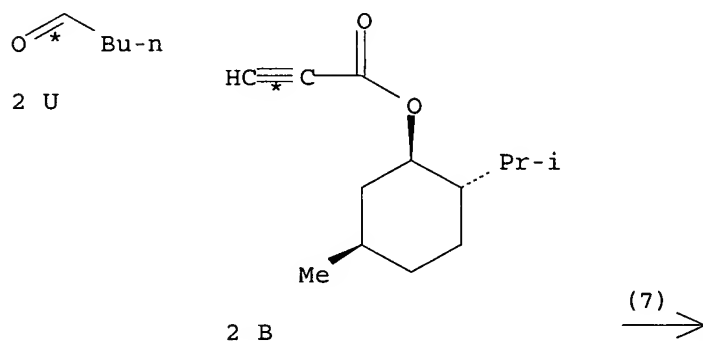
PRO M 597583-79-4  
NTE stereoselective

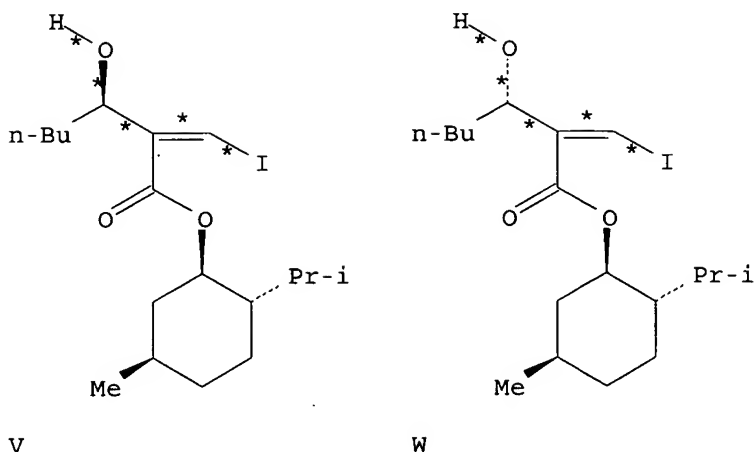
AN 139:245432 CASREACT  
TI Stereoselective aldol coupling of  $\alpha,\beta$ -acetylenic ketones promoted by MgI2  
AU Wei, Han-Xun; Hu, Jiali; Purkiss, David W.; Pare, Paul W.  
CS Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX, 79409, USA  
SO Tetrahedron Letters (2003), 44(5), 949-952  
CODEN: TELEAY; ISSN: 0040-4039  
PB Elsevier Science B.V.  
DT Journal  
LA English  
AB A highly stereoselective synthesis of (Z)- $\beta$ -iodovinyl ketone was achieved with the tandem formation of C-C and C-I bonds in a three-component reaction. This new catalysis utilizes MgI2 as a Lewis acid as well as an iodine source for a Michael-type addition  $\alpha,\beta$ -Acetylenic ketone is initially converted to an active  $\beta$ -iodo allenolate intermediate and then can be attacked by a variety of aldehydes to afford Z-selective Baylis-Hillman adducts in excellent yields.

RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 12 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(7) OF 9 2 U + 2 B ==> V + W





RX(7) RCT U 110-62-3, B 65018-52-2

STAGE(1)

RGT E 10377-58-9 MgI2  
SOL 75-09-2 CH2Cl2  
CON 18 hours, 0 deg C

STAGE(2)

RGT F 144-55-8 NaHCO3  
SOL 7732-18-5 Water

PRO V 587833-53-2, W 587833-54-3

NTE stereoselective, 82% overall yield

AN 139:214175 CASREACT

TI Asymmetric synthesis of chiral  $\beta$ -iodo Baylis-Hillman esters using MgI2 as promoter via a one-pot three-component reaction

AU Wei, Han-Xun; Chen, Dianjun; Xu, Xin; Li, Guigen; Pare, Paul W.

CS Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX, 79409-1061, USA

SO Tetrahedron: Asymmetry (2003), 14(8), 971-974

CODEN: TASYE3; ISSN: 0957-4166

PB Elsevier Science Ltd.

DT Journal

LA English

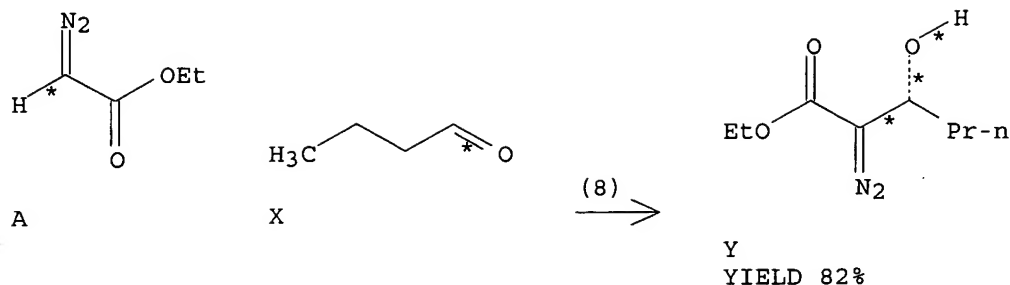
AB An asym. synthesis of  $\beta$ -iodo- $\alpha$ -(hydroxyalkyl)acrylates has been developed involving conjugate addition of I- to menthyl propiolates to give  $\beta$ -iodo allenolate intermediates, which undergo 1,2-addition to form  $\beta$ -iodo Baylis-Hillman products. Modest diastereoselectivities (37-58% de) and excellent yields (80-87%) were obtained when (1R,2S,5R)-(-)-menthol was used as a chiral auxiliary. The two diastereoisomers of the product were separated by silica gel chromatog. to give diastereomerically pure products.

RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 13 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(8) OF 14 A + X ==> Y





RX(8)

## STAGE(1)

CAT 18531-94-7 (R)-2,2'-Binaphthol, 1071-76-7 1-Butanol,  
zirconium(4+) salt  
SOL 110-71-4 (CH<sub>2</sub>OMe)<sub>2</sub>  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) 1 hour, room temperature

## STAGE(2)

RCT A 623-73-4  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) room temperature  
SUBSTAGE(3) 3 hours, room temperature

## STAGE(3)

RCT X 123-72-8  
RGT N 7789-48-2 MgBr<sub>2</sub>  
CON SUBSTAGE(3) 3 days

PRO Y 529477-85-8  
NTE stereoselective

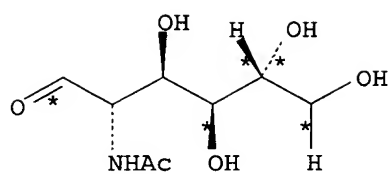
AN 138:401243 CASREACT  
TI Direct Catalytic Asymmetric Aldol-Type Reaction of Aldehydes with Ethyl  
Diazoacetate  
AU Yao, Wengang; Wang, Jianbo  
CS College of Chemistry, Key Laboratory of Bioorganic Chemistry and Molecular  
Engineering of Ministry of Education, Department of Chemical Biology,  
Peking University, Beijing, 100871, Peop. Rep. China  
SO Organic Letters (2003), 5(9), 1527-1530  
CODEN: ORLEF7; ISSN: 1523-7060  
PB American Chemical Society  
DT Journal  
LA English  
AB The direct aldol-type condensation of aldehydes with Et diazoacetate  
catalyzed by the chiral complex of BINOL derivs.-Zr(OCMe<sub>3</sub>)<sub>4</sub> gave  
β-hydroxy α-diazo carbonyl compds. with moderate  
enantioselectivities (53-87% ee).  
RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 14 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

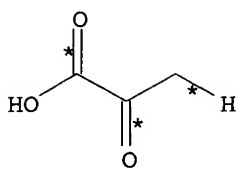
RX(3) OF 3 COMPOSED OF RX(1), RX(2)

RX(3) A + B + C + D + I ==> J

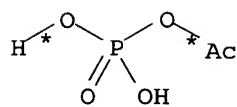
Prepared by: Mary Hale @2-2507 Rem Bldg 1D86



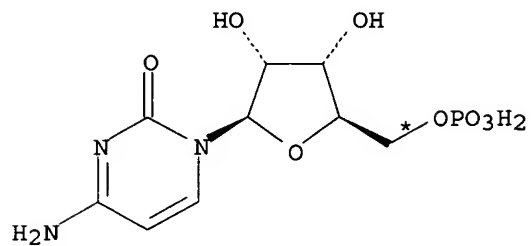
A



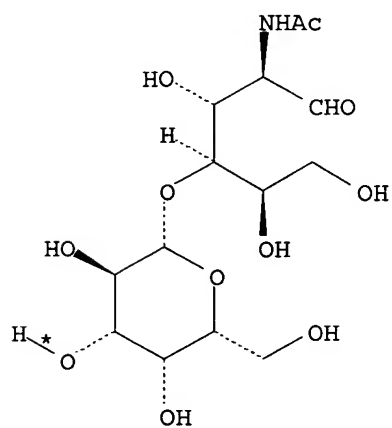
B



C

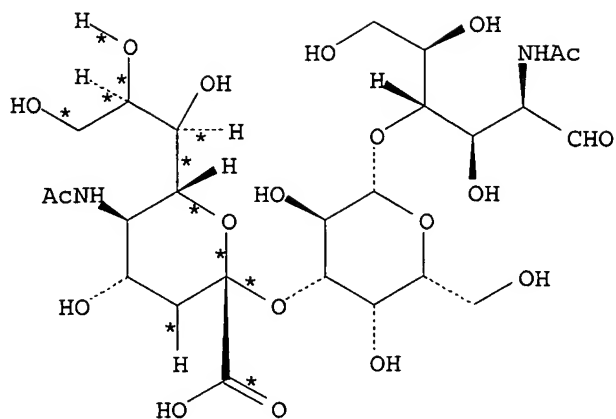


D



I

2  
STEPS  
→



J

RX(1) RCT A 3615-17-6, B 127-17-3, C 590-54-5, D 63-37-6  
 RGT F 7786-30-3 MgCl<sub>2</sub>  
 PRO E 3063-71-6  
 CAT 56-65-5 Adenosine 5'-(tetrahydrogen triphosphate)  
 SOL 7732-18-5 Water  
 CON 4 hours, 37 deg C, pH 8  
 NTE biotransformation, recombinant Escherichia coli whole cells or cell ext. used, Tris-buffered soln. used

RX(2) RCT E 3063-71-6, I 32181-59-2  
 RGT F 7786-30-3 MgCl<sub>2</sub>  
 PRO J 81693-22-3  
 CAT 71124-51-1 Sialyltransferase, cytidine monophosphoacetylneuraminate- $\beta$ -galactoside  $\alpha$ 2 $\rightarrow$ 3-  
 SOL 7732-18-5 Water  
 CON 9 hours, 37 deg C, pH 7.6  
 NTE biotransformation, enzymic, recombinant Escherichia coli cell ext. used, Tris-buffered soln. used

AN 138:286050 CASREACT  
 TI Production of cytidine 5'-monophosphate N-acetylneuraminic acid using recombinant Escherichia coli as a biocatalyst  
 AU Lee, Sun-Gu; Lee, Jeong-Oh; Yi, Jung-Kyu; Kim, Byung-Gee  
 CS Institute of Molecular Biology and Genetics, School of Chemical Engineering, Seoul National University, Seoul, 151-742, S. Korea  
 SO Biotechnology and Bioengineering (2002), 80(5), 516-524  
 CODEN: BIBIAU; ISSN: 0006-3592  
 PB John Wiley & Sons, Inc.  
 DT Journal  
 LA English  
 AB An Escherichia coli strain expressing three recombinant enzymes, i.e., CMP (CMP) kinase, sialic acid aldolase and CMP N-acetylneuraminic acid (CMP-NeuAc) synthetase, was utilized as a biocatalyst for the production of CMP-NeuAc. Both recombinant E. coli extract and whole cells catalyzed the production of CMP-NeuAc from CMP (20 mM), N-acetylmannosamine (40 mM), pyruvate (60 mM), ATP (1 mM), and acetylphosphate (60 mM), resulting in 90% conversion yield based on initial CMP concentration used. It was confirmed that endogenous acetate kinase can catalyze not only the ATP regeneration in the conversion of CMP to CDP but also the conversion of CDP to CTP. On

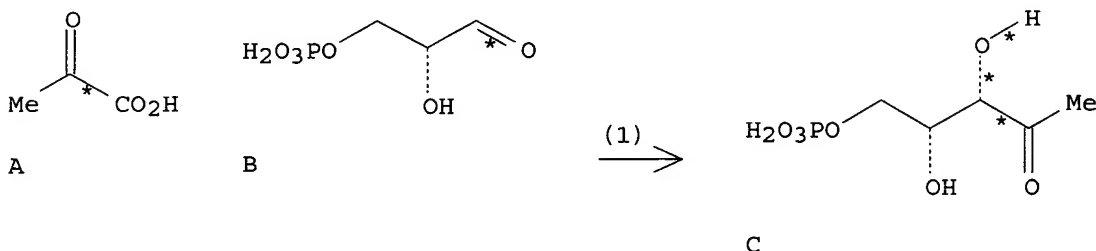
the other hand, endogenous pyruvate kinase and polyphosphate kinase could not regenerate ATP efficiently. The addition of exogenous acetate kinase to the reaction mixture containing the cell extract increased the conversion rate of

CMP to CMP-NeuAc by about 1.5-fold, but the addition of exogenous inorg. pyrophosphatase had no influence on the reaction. This E. coli strain could also be employed as an enzyme source for in situ regeneration of CMP-NeuAc in a sialyltransferase catalyzed reaction. About 90% conversion yield of  $\alpha$ 2,3-sialyl-N-acetylglactosamine was obtained from N-acetylglactosamine (20 mM), CMP (2 mM), N-acetylmannosamine (40 mM), pyruvate (60 mM), ATP (1 mM), and acetyl phosphate (80 mM) using the recombinant E. coli extract and  $\alpha$ 2,3-sialyltransferase.

RE.CNT 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 15 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(1) OF 3 A + B ==> C



RX(1) RCT A 127-17-3, B 591-57-1  
RGT D 202218-79-9 Synthetase, 1-deoxy-D-xylulose 5-phosphate, E 1185-53-1 (HOCH<sub>2</sub>)<sub>3</sub>CNH<sub>2</sub>.HCl, F 7786-30-3 MgCl<sub>2</sub>, G 154-87-0 Thiazolium, 3-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-4-methyl-5-(4,6,6-trihydroxy-4,6-dioxido-3,5-dioxa-4,6-diphosphahex-1-yl)-, chloride, H 113-24-6 Propanoic acid, 2-oxo-, sodium salt  
PRO C 190079-18-6  
SOL 7732-18-5 Water  
CON SUBSTAGE(1) 4 hours, 37 deg C  
SUBSTAGE(2) 10 minutes, 100 deg C  
NTE biotransformation, enzymic, stereoselective, buffered soln.  
AN 138:170418 CASREACT  
TI Enzymatic synthesis of 1-deoxysugar-phosphates using E. coli 1-deoxy-D-xylulose 5-phosphate synthase  
AU Querol, Jordi; Grosdemange-Billiard, Catherine; Rohmer, Michel; Boronat, Albert; Imperial, Santiago  
CS Facultat de Quimica, Departament de Bioquimica i Biologia Molecular, Universitat de Barcelona, Barcelona, 08028, Spain  
SO Tetrahedron Letters (2002), 43(46), 8265-8268  
CODEN: TELEAY; ISSN: 0040-4039  
PB Elsevier Science Ltd.  
DT Journal  
LA English  
AB The thiamine diphosphate-dependent enzyme 1-deoxy-D-xylulose 5-phosphate synthase from Escherichia coli can use D-erythrose 4-phosphate and D-ribose 5-phosphate as alternative substrates. These reactions were used for the production of 1-deoxy-D-fructose 6-phosphate and 1-deoxy-D-

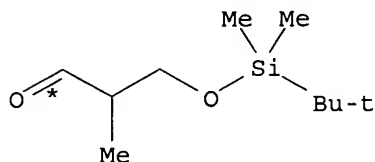
sedoheptulose 7-phosphate and have potential application for the biosynthesis of other 1-deoxysugar phosphates.

RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

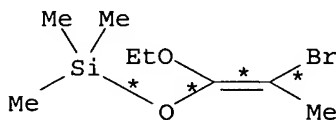
L6 ANSWER 16 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(8) OF 28 COMPOSED OF RX(1), RX(2)

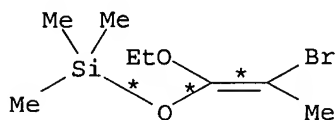
RX(8) 2 A + 2 B ==> G



2 A

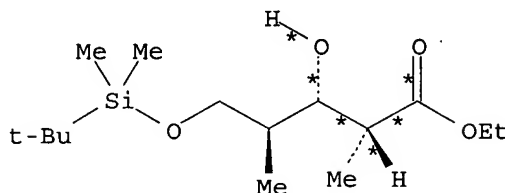


B



B

2  
STEPS  
→



G  
YIELD 80%

RX(1) RCT A 91751-25-6, B 153645-08-0  
PRO C 374896-36-3, D 374896-37-4  
CAT 177274-09-8 1,3,2-Oxazaborolidin-5-one, 4-(1-methylethyl)-3-[(4-methylphenyl)sulfonyl]-, (4R)-  
SOL 75-09-2 CH2Cl2

RX(2) RCT C 374896-36-3  
RGT H 688-73-3 Bu3SnH, I 97-94-9 Et3B, J 7789-48-2 MgBr2  
PRO G 475051-45-7  
SOL 75-09-2 CH2Cl2

AN 137:369862 CASREACT

TI A short synthesis of the C15-C21 segment of (+)-discodermolide, based on an asymmetric approach from achiral 2-methyl-1,3-propanediol to versatile enantiopure stereotriads

AU Shahid, Kazi A.; Li, Yong-Nan; Okazaki, Momotoshi; Shuto, Yoshihiro; Goto, Fumitaka; Kiyooka, Syun-ichi

CS The United Graduate School of Agricultural Sciences, Ehime University, Tarumi, Matsuyama, 790-8566, Japan

SO Tetrahedron Letters (2002), 43(36), 6373-6376

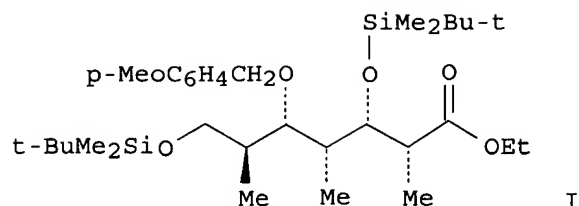
CODEN: TELEAY; ISSN: 0040-4039

PB Elsevier Science Ltd.

DT Journal

LA English

GI



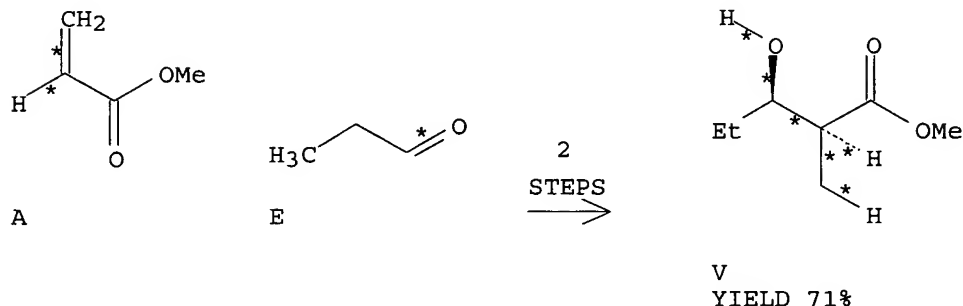
AB A new approach was developed to versatile enantiopure stereotriads using chiral oxazaborolidinone-promoted asym. aldol reaction of a racemic aldehyde with a bromo silyl nucleophile. A short synthesis of the C15-C21 segment I of (+)-discodermolide was achieved by elongation of one of the stereotriads with further diastereoselective aldol reaction with the same nucleophile.

RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 17 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(24) OF 29 COMPOSED OF RX(2), RX(9)

RX(24) A + E ==> V



RX(2) RCT A 96-33-3, E 123-38-6  
RGT D 280-57-9 Triethylenediamine  
PRO F 18052-21-6  
NTE regioselective

RX(9) RCT F 18052-21-6

STAGE(1)

RGT S 7789-48-2 MgBr<sub>2</sub>  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

STAGE(2)

RGT T 1333-74-0 H<sub>2</sub>  
CAT 7440-05-3 Pd

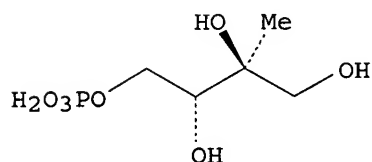
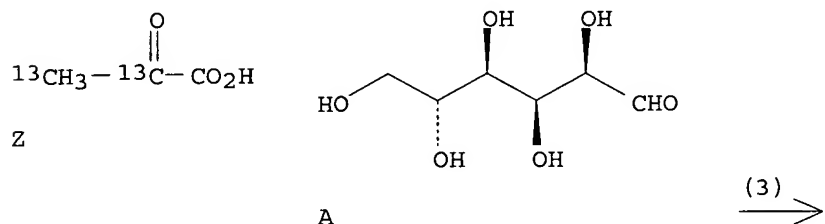
PRO V 67498-21-9

NTE stereoselective, in the absence of MgBr<sub>2</sub> no stereoselectivity found

AN 136:369262 CASREACT  
 TI Magnesium Bromide Mediated Highly Diastereoselective Heterogeneous Hydrogenation of Olefins  
 AU Bouzide, Abderrahim  
 CS INRS-Institut Armand Frappier, Laval, QC, H7V 1B7, Can.  
 SO Organic Letters (2002), 4(8), 1347-1350  
 CODEN: ORLEF7; ISSN: 1523-7060  
 PB American Chemical Society  
 DT Journal  
 LA English  
 AB Palladium on carbon combined with magnesium bromide catalyzed hydrogenation of Baylis-Hillman olefins to afford the corresponding aldol derivs. in a highly syn-diastereoselective manner is described.  
 RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 18 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(3) OF 5 Z + A ==> AA



AA  
 YIELD 50%

RX(3) RCT Z 127350-53-2, A 19030-38-7

STAGE(1)

RGT D 7786-30-3 MgCl<sub>2</sub>, F 154-87-0 Thiazolium, 3-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-4-methyl-5-(4,6,6-trihydroxy-4,6-dioxido-3,5-dioxo-4,6-diphosphahex-1-yl)-, chloride, G 1310-73-2 NaOH, AB 56-65-5 Adenosine 5'-(tetrahydrogen triphosphate)  
 CAT 9023-78-3 Isomerase, triose phosphate, 9001-51-8 Kinase (phosphorylating), hexo-, 9001-41-6 Isomerase, glucose phosphate, 9001-80-3 Kinase (phosphorylating), phosphofructo-, 9024-52-6 Fructoaldolase, 202218-79-9 Synthetase, 1-deoxy-D-xylulose 5-phosphate

SOL 7732-18-5 Water

## STAGE(2)

RGT AC 7647-01-0 HCl

SOL 7732-18-5 Water

## STAGE(3)

RGT H 50-99-7 D-Glucose

CAT 210756-42-6 Isomerase, 1-deoxy-D-xylulose 5-phosphate reducto-, 37250-50-3 Dehydrogenase, glucose (nicotinamide adenine dinucleotide phosphate), 53-59-8 Coenzyme II

PRO AA 275826-87-4

NTE enzymic, biotransformation, buffered soln.

AN 136:70022 CASREACT

TI Biosynthesis of Terpenoids: Efficient Multistep Biotransformation Procedures Affording Isotope-Labeled 2C-Methyl-D-erythritol 4-Phosphate Using Recombinant 2C-Methyl-D-erythritol 4-Phosphate Synthase

AU Hecht, Stefan; Wungsintaweekul, Juraithip; Rohdich, Felix; Kis, Klaus; Radykewicz, Tanja; Schuhr, Christoph A.; Eisenreich, Wolfgang; Richter, Gerald; Bacher, Adelbert

CS Lehrstuhl fuer Organische Chemie und Biochemie, Technische Universitaet Muenchen, Garching, D-85747, Germany

SO Journal of Organic Chemistry (2001), 66(23), 7770-7775

CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

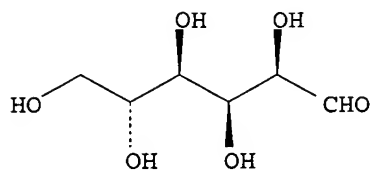
LA English

AB This paper describes the recombinant expression of the ispC gene of Escherichia coli specifying 2C-methyl-D-erythritol 4-phosphate synthase in a modified form that can be purified efficiently by metal-chelating chromatog. The enzyme was used for the preparation of isotope-labeled 2C-methyl-D-erythritol 4-phosphate employing isotope-labeled glucose and pyruvate as starting materials. The simple one-pot methods described afford numerous isotopomers of 2C-methyl-D-erythritol 4-phosphate carrying 3H, 13C, or 14C from com. available precursors. The overall yield based on the resp. isotope-labeled starting material is approx. 50%.

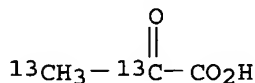
RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 19 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

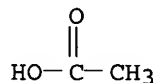
RX(1) OF 3 A + B + C ==&gt; D



A

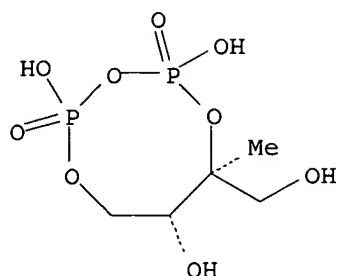
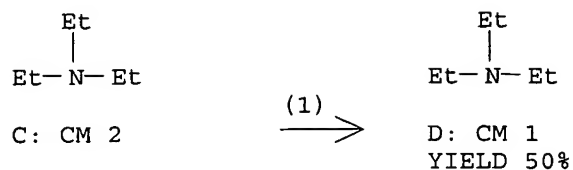


B



C: CM 1





D: CM 2  
YIELD 50%

RX(1) RCT A 19030-38-7, B 127350-53-2

STAGE(1)

RGT E 7786-30-3 MgCl<sub>2</sub>, F 56-65-5 Adenosine  
5'-(tetrahydrogen triphosphate), G 154-87-0 Thiazolium,  
3-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-4-methyl-5-  
(4,6,6-trihydroxy-4,6-dioxido-3,5-dioxo-4,6-diphosphahex-1-  
yl)-, chloride, H 1310-73-2 NaOH  
CAT 9001-51-8 Kinase (phosphorylating), hexo-, 9001-40-5  
Dehydrogenase, glucose 6-phosphate, 9001-80-3 Kinase  
(phosphorylating), phosphofructo-, 9024-52-6  
Fructoaldolase, 9023-78-3 Isomerase, triose phosphate,  
210756-42-6 Isomerase, 1-deoxy-D-xylulose 5-phosphate  
reducto-  
SOL 7732-18-5 Water

STAGE(2)

RGT I 50-99-7 D-Glucose, J 53-59-8 Coenzyme II  
CAT 210756-42-6 Isomerase, 1-deoxy-D-xylulose 5-phosphate  
reducto-, 9028-53-9 Dehydrogenase, glucose

STAGE(3)

RGT K 3483-12-3 Cleland's reagent, L 65-47-4 Cytidine  
5'-(tetrahydrogen triphosphate), M 138-08-9  
Phosphoenolpyruvate, N 7647-01-0 HCl  
CAT 9026-50-0 Kinase (phosphorylating), nucleoside  
monophosphate, 9026-51-1 Kinase (phosphorylating),  
nucleoside diphosphate, 9001-59-6 Kinase (phosphorylating),  
pyruvate, 251990-59-7 Cytidylyltransferase,  
2-C-methylerythritol 4-, 263016-77-9 Kinase  
(phosphorylating), 4-diphosphocytidyl-2-C-methylerythritol  
2-, 287480-92-6 Synthase, 2-C-methyl-D-erythritol  
2,4-cyclodiphosphate  
SOL 7732-18-5 Water

## STAGE(4)

RCT C 5204-74-0  
SOL 7732-18-5 Water

PRO D 383126-41-8

NTE biotransformation, enzymic, stereoselective, buffered soln.

AN 136:70021 CASREACT

TI Studies on the non-mevalonate pathway - preparation and properties of isotope-labeled 2C-methyl-D-erythritol 2,4-cyclodiphosphate

AU Schuhr, Christoph A.; Hecht, Stefan; Kis, Klaus; Eisenreich, Wolfgang; Wungsintaweekul, Juraithip; Bacher, Adelbert; Rohdich, Felix

CS Lehrstuhl fur Organische Chemie und Biochemie, Technische Universitat Munchen, Garching, 85747, Germany

SO European Journal of Organic Chemistry (2001), (17), 3221-3226

CODEN: EJOCFK; ISSN: 1434-193X

PB Wiley-VCH Verlag GmbH

DT Journal

LA English

AB Recent studies have shown that 2C-methyl-D-erythritol 2,4-cyclodiphosphate can be formed from 2C-methyl-D-erythritol 4-phosphate by the consecutive action of IspD, IspE and IspF proteins in the non-mevalonate pathway of isoprenoid biosynthesis. We describe here rapid one-pot strategies for the enzyme-assisted preparation of this compound from isotope-labeled pyruvate and glucose that are optimized for the introduction of <sup>13</sup>C or <sup>14</sup>C and afford a wide variety of isotopomers in mmol quantity. The one-pot reactions involving up to 10 forward reaction steps and up to 15 enzyme catalysts have an overall yield of 50 to 80% of purified product.

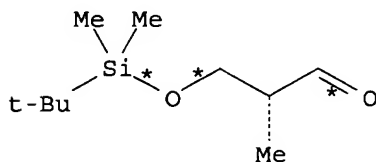
RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

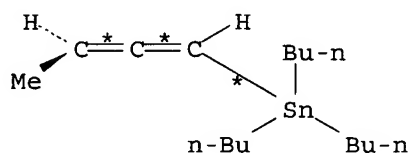
L6 ANSWER 20 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(346) OF 385 COMPOSED OF RX(17), RX(18), RX(19), RX(20), RX(21)

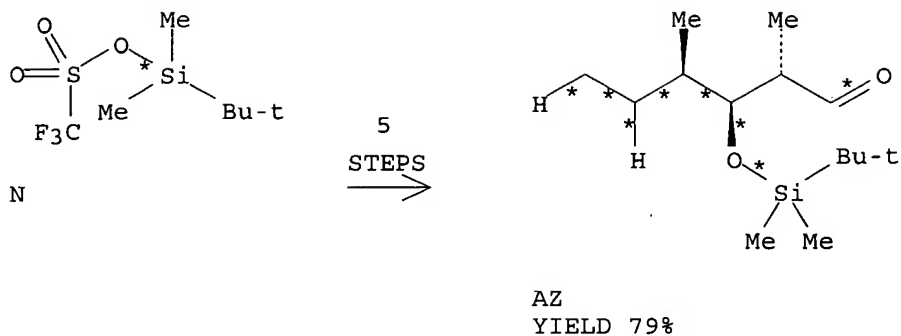
RX(346) J + AT + N ==&gt; AZ



J



AT



RX(17) RCT J 97826-89-6

STAGE(1)

RGT AV 29858-07-9 MgBr<sub>2</sub>-Et<sub>2</sub>O

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

STAGE(2)

RCT AT 202119-26-4

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

STAGE(3)

RGT I 7732-18-5 Water

PRO AU 289900-06-7

RX(18) RCT AU 289900-06-7, N 69739-34-0

STAGE(1)

RGT P 108-48-5 2,6-Lutidine

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

STAGE(2)

RGT F 144-55-8 NaHCO<sub>3</sub>

SOL 7732-18-5 Water

PRO AW 204448-51-1

RX(19) RCT AW 204448-51-1

RGT R 1333-74-0 H<sub>2</sub>

PRO AX 379732-73-7

CAT 7440-06-4 Pt

SOL 64-17-5 EtOH

NTE catalyst on carbon

RX(20) RCT AX 379732-73-7

STAGE(1)

CAT 24057-28-1 Pyridinium tosylate

SOL 64-17-5 EtOH, 7732-18-5 Water

STAGE(2)

RGT E 121-44-8 Et<sub>3</sub>N

PRO AY 379732-75-9

RX(21) RCT AY 379732-75-9

## STAGE(1)

RGT F 144-55-8 NaHCO<sub>3</sub>, AR 87413-09-0 Martin's reagent  
 SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

## STAGE(2)

RGT AS 7772-98-7 Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub>, F 144-55-8 NaHCO<sub>3</sub>  
 SOL 7732-18-5 Water

PRO AZ 379732-77-1

AN 136:37441 CASREACT

TI Synthesis of stereopentad analogs of the C14-C22 segment of callystatin A through additions of chiral allenylzinc reagents to stereotriads

AU Marshall, James A.; Schaaf, Gregory M.

CS Department of Chemistry, University of Virginia, Charlottesville, VA, 22904, USA

SO Journal of Organic Chemistry (2001), 66(23), 7825-7831  
CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

LA English

AB The addition of (P)- and (M)-allenylzinc reagents, prepared in situ through Pd-catalyzed metalation of (R)- and (S)-3-butyn-2-ol mesylates, to diastereomeric stereotriad aldehydes (2R,3R,4S)-, (2S,3R,4R)-, (2S,3S,4S)-, and (2R,3S,4R)-OHCCHMeCH(OSiMe<sub>2</sub>CMe<sub>3</sub>)CHMeCH<sub>2</sub>Me, of syn,syn, syn,anti, anti,anti, and anti,syn stereochem. was examined in order to prepare the C14-C22 segment of callystatin A. Addns. to the former two aldehydes afforded the four anti adducts with high diastereoselectivity and negligible mismatching. Significant mismatching was observed with the latter two aldehydes and the (M)-allenylzinc reagent. An evaluation of possible transition states is presented in consideration of steric and dipolar control elements.

RE.CNT 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

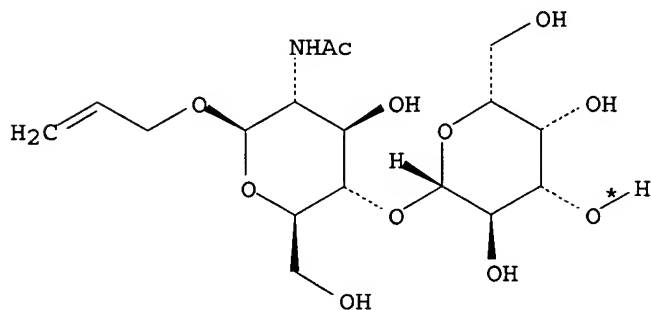
L6 ANSWER 21 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(86) OF 98 COMPOSED OF REACTION SEQUENCE RX(26), RX(27)

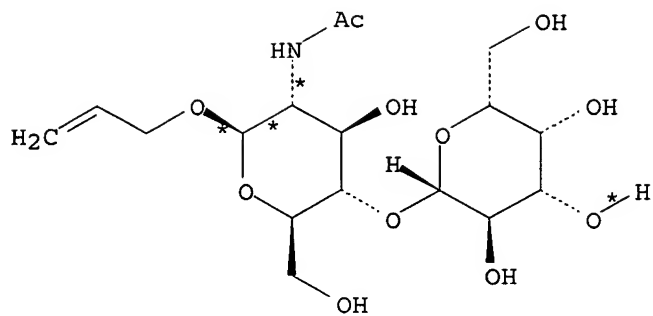
AND REACTION SEQUENCE RX(2), RX(1), RX(5), RX(4), RX(6), RX(27)

...3 BV + 3 CB ==&gt; CC...

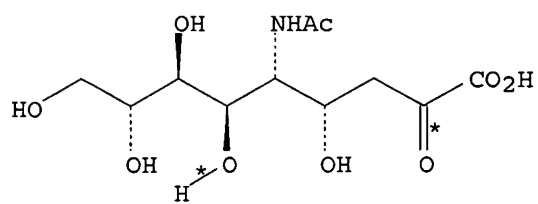
...4 I + 3 J + 3 X + 3 Y + 3 CC ==&gt; CE + CF + CG



2 BV

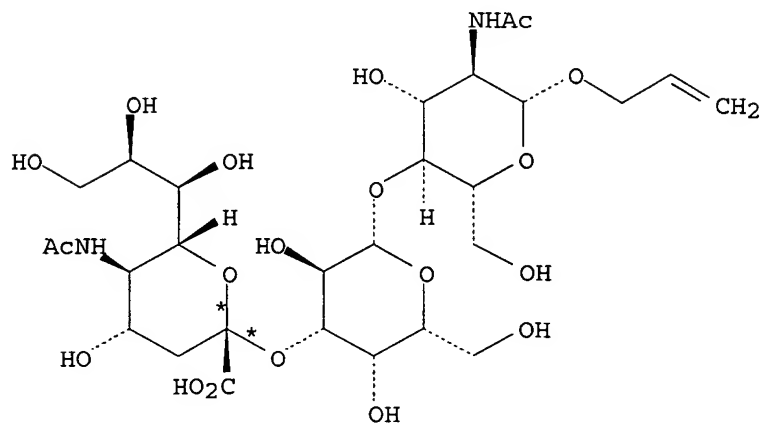


BV



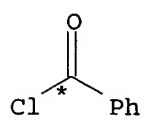
3 CB

6  
STEPS  
→

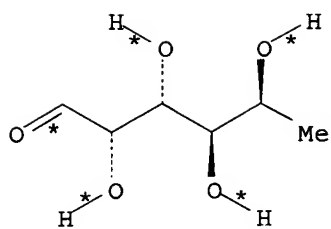


CC

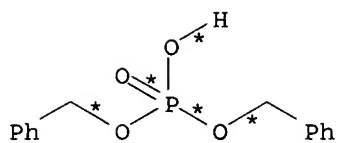
START NEXT REACTION SEQUENCE



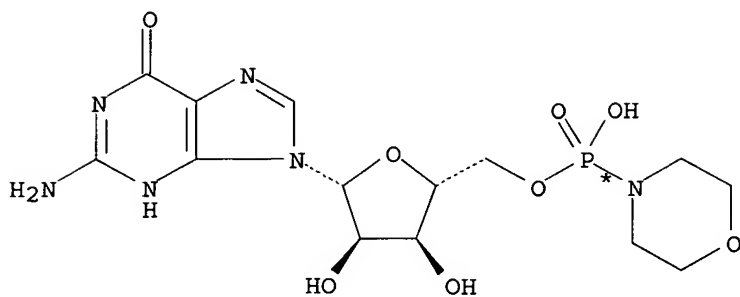
4 I



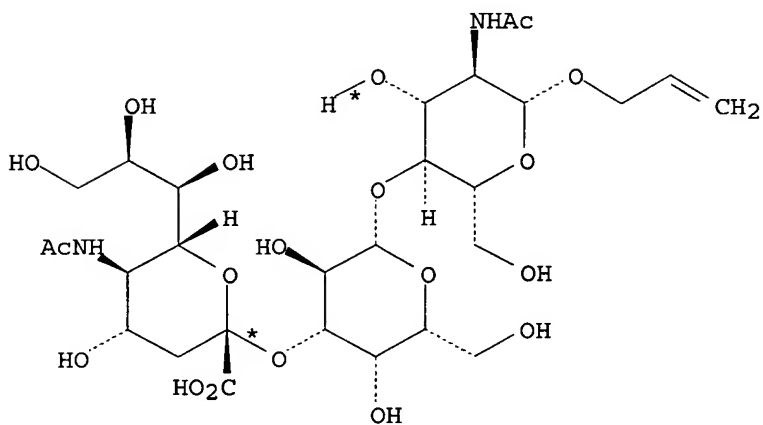
3 J



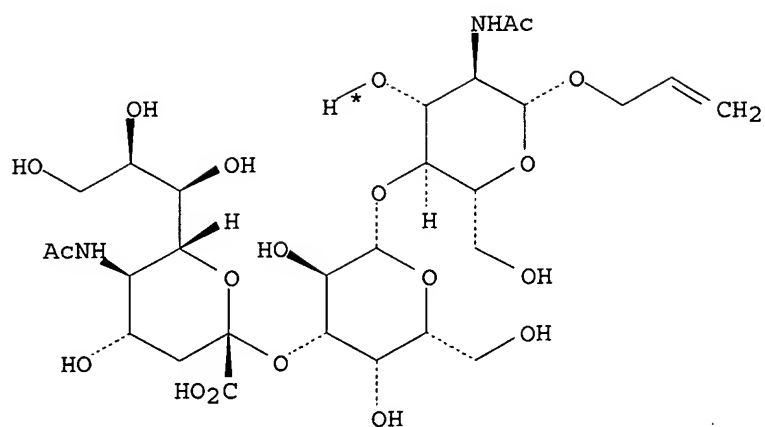
3 X



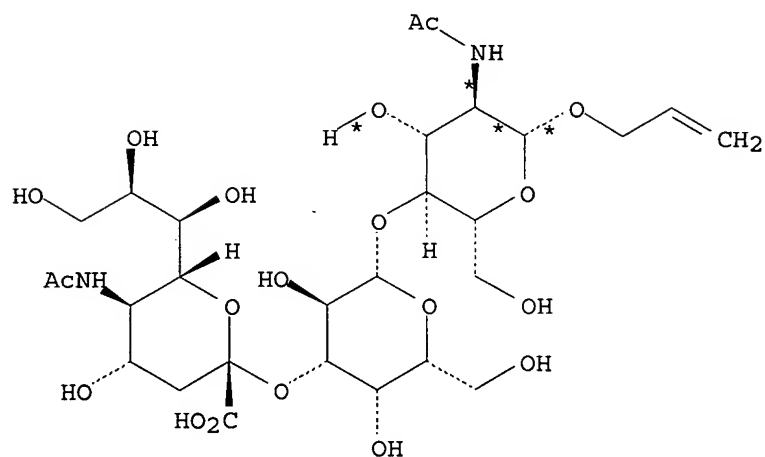
3 Y



CC



CC

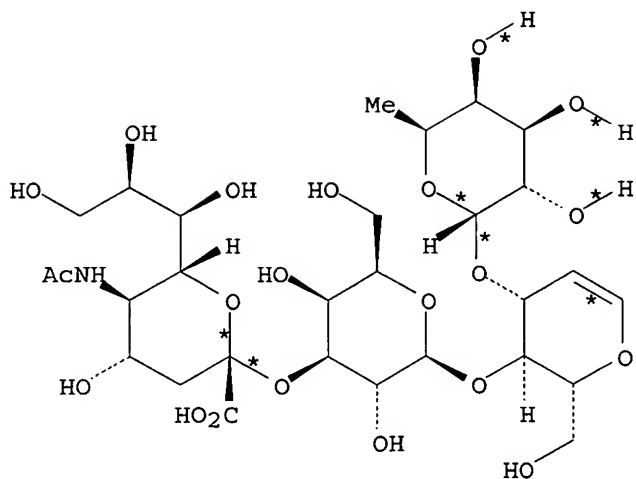


CC

6  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*



CG

RX(26) RCT BV 86733-47-3, CB 131-48-6  
 RGT BZ 7786-30-3 MgCl<sub>2</sub>, BY 7773-01-5 MnCl<sub>2</sub>, BD 7447-40-7  
 KCl, CD 56-65-5 Adenosine 5'-(tetrahydrogen triphosphate)  
 PRO CC 143398-10-1  
 NTE ENZYMIC ,STEREOSELECTIVE

RX(2) RCT I 98-88-4, J 2438-80-4

STAGE(1)  
 SOL 110-86-1 Pyridine

STAGE(2)  
 SOL 7732-18-5 Water

STAGE(3)  
 SOL 141-78-6 AcOEt

STAGE(4)  
 RGT C 108-24-7 Ac<sub>2</sub>O, D 10035-10-6 HBr  
 SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

STAGE(5)  
 SOL 7732-18-5 Water

STAGE(6)  
 SOL 141-78-6 AcOEt

STAGE(7)  
 RGT K 534-16-7 Ag<sub>2</sub>CO<sub>3</sub>  
 SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>, 60-29-7 Et<sub>2</sub>O, 75-05-8 MeCN

PRO A 140223-15-0  
 NTE STEREOSELECTIVE

RX(1) RCT A 140223-15-0

STAGE(1)



RGT C 108-24-7 Ac2O, D 10035-10-6 HBr, E 64-19-7 AcOH  
SOL 75-09-2 CH2Cl2

STAGE(2)  
SOL 7732-18-5 Water

STAGE(3)  
SOL 141-78-6 AcOEt

PRO B 131897-73-9  
NTE STEREOSELECTIVE

RX(5) RCT B 131897-73-9, X 1623-08-1  
RGT K 534-16-7 Ag2CO3  
PRO Q 138552-47-3  
SOL 75-09-2 CH2Cl2, 60-29-7 Et2O, 75-05-8 MeCN  
NTE STEREOSELECTIVE, Mol. SIEVES USED

RX(4) RCT Q 138552-47-3

STAGE(1)  
RGT S 144-55-8 NaHCO3, T 1333-74-0 H2  
CAT 7440-05-3 Pd  
SOL 64-17-5 EtOH

STAGE(2)  
RGT U 1310-73-2 NaOH  
SOL 7732-18-5 Water

STAGE(3)  
RGT E 64-19-7 AcOH

PRO R 16562-59-7  
NTE STEREOSELECTIVE

RX(6) RCT R 16562-59-7

STAGE(1)  
RGT AA 121-44-8 Et3N

STAGE(2)  
RGT AB 11114-15-1 DOWEX 50W  
SOL 7732-18-5 Water

STAGE(3)  
RCT Y 7390-53-6  
SOL 110-86-1 Pyridine

STAGE(4)  
SOL 7732-18-5 Water

PRO Z 15839-70-0  
NTE STEREOSELECTIVE, DOWEX 50W-X8 USED

RX(27) RCT CC 143398-10-1, Z 15839-70-0  
RGT BY 7773-01-5 MnCl2, CD 56-65-5 Adenosine 5'-(tetrahydrogen triphosphate)  
PRO CE 143398-11-2, CF 141612-83-1, CG 142800-36-0  
NTE BUFFERED SOLN., STEREOSELECTIVE  
AN 136:4799 CASREACT

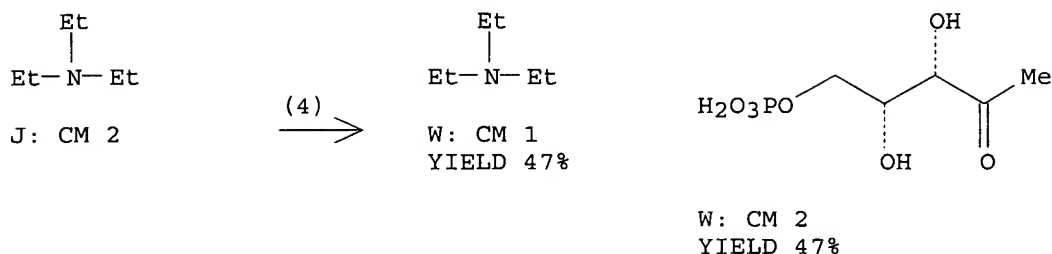
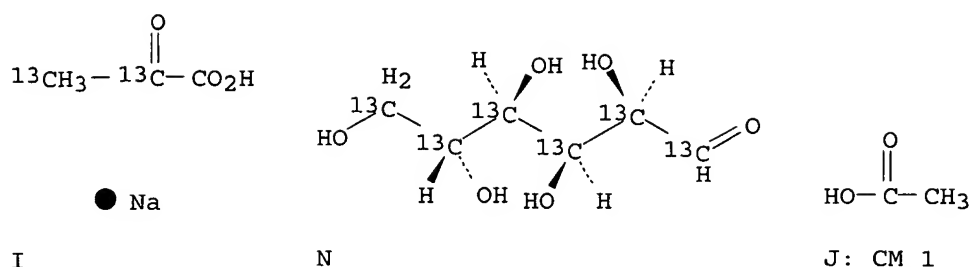
TI Production of fucosylated carbohydrates by enzymatic fucosylation  
 synthesis of sugar nucleotides; and in situ regeneration of GDP-fucose  
 IN Wong, Chi-huey; Ichikawa, Yoshitaka; Shen, Gwo-jenn; Liu, Kun-chin  
 PA Scripps Research Institute, USA  
 SO U.S., 45 pp., Cont.-in-part of U.S. Ser. No. 910,612, abandoned.  
 CODEN: USXXAM

DT Patent  
 LA English  
 FAN.CNT 8

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6319695	B1	20011120	US 1992-961076	19921014
	WO 9308205	A1	19930429	WO 1992-US8789	19921015
	W: AU, BB, BG, BR, CA, CS, FI, HU, JP, KP, KR, LK, MG, MN, MW, NO, PL, RO, RU, SD				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG				
	AU 9227854	A1	19930521	AU 1992-27854	19921015
	AU 675209	B2	19970130		
	JP 07500248	T2	19950112	JP 1992-507791	19921015
	EP 642526	A1	19950315	EP 1992-921939	19921015
	EP 642526	B1	19981223		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, SE				
	HU 69791	A2	19950928	HU 1994-1072	19921015
	AT 174925	E	19990115	AT 1992-921939	19921015
	ES 2129458	T3	19990616	ES 1992-921939	19921015
	CA 2121365	C	20001128	CA 1992-2121365	19921015
	RO 118132	B1	20030228	RO 1994-636	19921015
	US 6518418	B1	20030211	US 1992-991182	19921210
	FI 9401732	A	19940614	FI 1994-1732	19940414
	NO 9401346	A	19940614	NO 1994-1346	19940414
	US 2002068331	A1	20020606	US 2001-992680	20011119
PRAI	US 1991-777662		19911015		
	US 1992-901260		19920619		
	US 1992-910612		19920708		
	US 1992-961076		19921014		
	WO 1992-US8789		19921015		
AB	This invention contemplates improved methods of enzymic production of carbohydrates especially fucosylated carbohydrates. Improved syntheses of glycosyl 1- or 2-phosphates using both chemical and enzymic means are also contemplated. The phosphorylated glycosides are then used to produce sugar nucleotides that are in turn used as donor sugars for glycosylation of acceptor carbohydrates. Especially preferred herein is the use of a disclosed method for fucosylation.				
RE.CNT	37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT				

L6 ANSWER 22 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(4) OF 6 I + N + J ==> W



RX(4) RCT I 89196-78-1, N 110187-42-3

STAGE(1)

RGT P 7786-30-3  $\text{MgCl}_2$ , E 136-09-4 Thiazolium,  
 3-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-4-methyl-5-  
 (4,6,6-trihydroxy-4,6-dioxido-3,5-dioxo-4,6-diphosphahex-1-  
 yl)-, inner salt, Q 987-65-5 Adenosine 5'-(tetrahydrogen  
 triphosphate), disodium salt  
 CAT 202218-79-9 Synthetase, 1-deoxy-D-xylulose 5-phosphate,  
 9001-51-8 Kinase (phosphorylating), hexo-, 9001-41-6  
 Isomerase, glucose phosphate, 9001-80-3 Kinase  
 (phosphorylating), phosphofructo-, 9024-52-6 Fructoaldolase  
 SOL 7732-18-5 Water

STAGE(2)

RCT J 5204-74-0  
 SOL 7732-18-5 Water

PRO W 346712-81-0

NTE buffered soln., biotransformation, enzymic

AN 135:77022 CASREACT

TI Enzyme-Assisted Preparation of Isotope-Labeled 1-Deoxy-D-xylulose 5-Phosphate

AU Hecht, Stefan; Kis, Klaus; Eisenreich, Wolfgang; Amslinger, Sabine;  
 Wungsintaweeikul, Juraithip; Herz, Stefan; Rohdich, Felix; Bacher, Adelbert  
 CS Lehrstuhl fuer Organische Chemie und Biochemie, Technische Universitaet  
 Muenchen, Garching, D-85747, Germany

SO Journal of Organic Chemistry (2001), 66(11), 3948-3952  
 CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

LA English

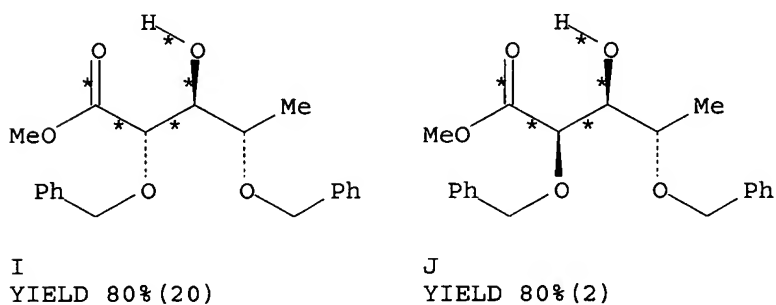
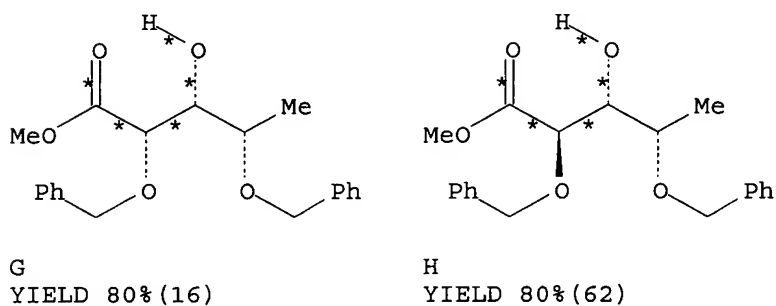
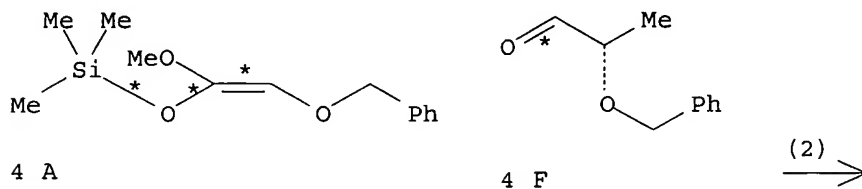
AB Recombinant 1-deoxy-D-xylulose 5-phosphate synthase of *Bacillus subtilis*  
 was used for the preparation of isotope-labeled 1-deoxy-D-xylulose 5-phosphate

using isotope-labeled glucose and/or isotope-labeled pyruvate as starting materials. The simple one-pot methods described afford almost every conceivable isotopomer of 1-deoxy-D-xylulose 5-phosphate carrying  $^{13}\text{C}$  or  $^{14}\text{C}$  from com. available precursors with an overall yield around 50%.

RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 23 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(2) OF 2 4 A + 4 F ==> G + H + I + J



RX(2) RCT A 139400-25-2, F 81445-44-5

STAGE(1)

RGT D 29858-07-9  $\text{MgBr}_2 \cdot \text{Et}_2\text{O}$   
SOL 108-88-3 PhMe

STAGE(2)

RGT K 12408-02-5  $\text{H}^+$

PRO G 97416-48-3, H 97416-47-2, I 97416-45-0, J 97416-46-1

NTE stereoselective, yield and ratio related activator

AN 134:366381 CASREACT

TI Magnesium bromide diethyl etherate mediated highly diastereoselective aldol reaction between an aldehyde and a silyl enol ether

AU Fujisawa, Hidehiko; Sasaki, Yasuhiro; Mukaiyama, Teruaki

CS Department of Applied Chemistry, Faculty of Science, Science University of Tokyo, Tokyo, 162-8601, Japan

SO Chemistry Letters (2001), (3), 190-191

CODEN: CMLTAG; ISSN: 0366-7022

PB Chemical Society of Japan

DT Journal

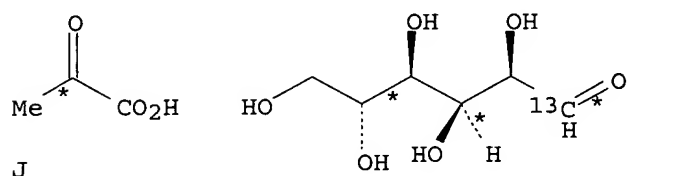
LA English

AB High yield and excellent diastereoselectivity in the formation of products in magnesium bromide-diethyl etherate promoted aldol reactions was reported. For example, the reaction of 2-deoxy-5-O-[(1,1-dimethylethyl)dimethylsilyl]-3-O-[(4-methoxyphenyl)methyl]-2,2-dimethyl-4-O-(phenylmethyl)-L-erythro-pentose with [(1Z)-1-methoxy-2-(phenylmethoxy)ethenyl]oxy]trimethylsilane gave 4-deoxy-7-O-[(1,1-dimethylethyl)dimethylsilyl]-5-O-[(4-methoxyphenyl)methyl]-4,4-dimethyl-2,6-bis-O-(phenylmethyl)-manno-heptonic acid Me ester in 95% yield under optimized conditions. The following mechanism of the above aldol reaction proposes that magnesium bromide etherate activated both chiral alkoxy aldehydes and silyl enolate, i.e., magnesium enolate, formed by transmetalation from silyl enolate and  $\text{MgBr}_2 \cdot \text{OEt}_2$ , reacted with  $\text{MgBr}_2 \cdot \text{OEt}_2$ -chelated alkoxy aldehydes via the six-membered cyclic transition state.

RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

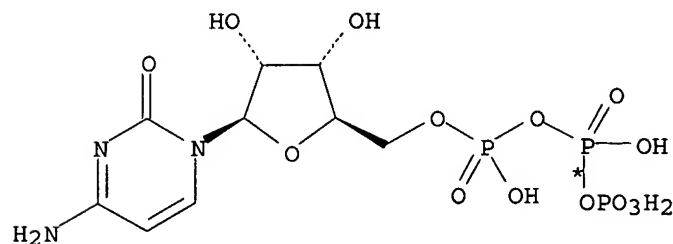
L6 ANSWER 24 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(6) OF 6 J + K + B ==&gt; U



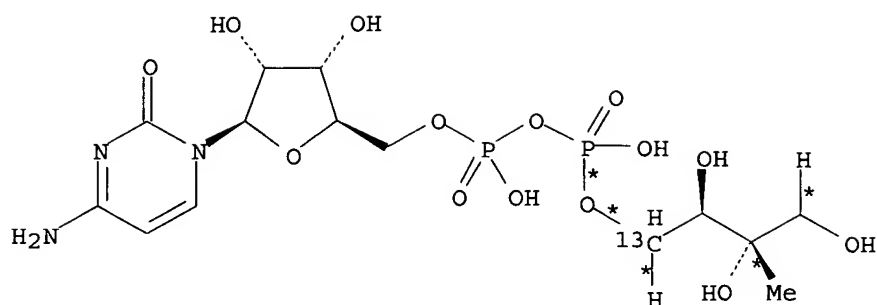
J

K



B

(6) →



U

RX(6) RCT J 127-17-3, K 40762-22-9

STAGE(1)

RGT V 84270-10-0 D-Glucose-4-13C, E 7786-30-3  
MgCl2, F 136-09-4 Thiazolium, 3-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-4-methyl-5-(4,6,6-trihydroxy-4,6-dioxido-3,5-dioxo-4,6-diphosphahex-1-yl)-, inner salt, G 56-65-5 Adenosine 5'-(tetrahydrogen triphosphate)

STAGE(2)

RGT H 1310-73-2 NaOH

STAGE(3)

RGT H 1310-73-2 NaOH

STAGE(4)

RGT I 307932-29-2 1,4-Dioxane-2,5-dimethanol, 2,5-diethoxy-, bis(dihydrogen phosphate), barium salt (1:4), E 7786-30-3 MgCl2

STAGE(5)

RCT B 65-47-4  
RGT H 1310-73-2 NaOH

PRO U 307932-32-7

AN 133:362928 CASREACT

TI Biosynthesis of Isoprenoids. A Rapid Method for the Preparation of Isotope-Labeled 4-Diphosphocytidyl-2C-methyl-D-erythritol

AU Rohdich, Felix; Schuhr, Christoph A.; Hecht, Stefan; Herz, Stefan; Wungsintaweekul, Juraithip; Eisenreich, Wolfgang; Zenk, Meinhard H.; Bacher, Adelbert

CS Lehrstuhl fuer Organische Chemie und Biochemie, Technische Universitaet Muenchen, Garching, D-85747, Germany

SO Journal of the American Chemical Society (2000), 122(40), 9571-9574  
CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

DT Journal

LA English

AB 4-Diphosphocytidyl-2C-methyl-D-erythritol serves as an intermediate in the non-mevalonate pathway of isoprenoid biosynthesis. The compound has been prepared in millimole quantity by a sequence of one-pot reactions using 13C-labeled pyruvate and dihydroxyacetone phosphate or 13C-labeled glucose as starting materials and recombinant enzymes of the non-mevalonate

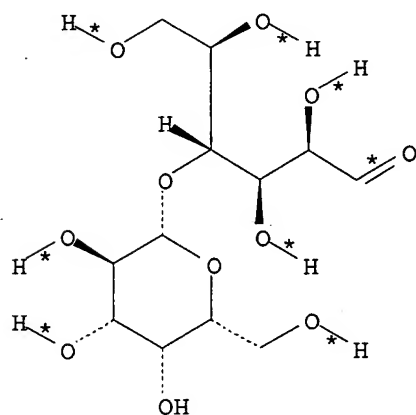
isoprenoid pathway as catalysts. The method has been used for the preparation of various 4-diphosphocytidyl-2C-methyl-D-erythritol isotopomers in high yield.

RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

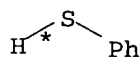
L6 ANSWER 25 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(63) OF 66 COMPOSED OF RX(1), RX(2), RX(5), RX(9), RX(10), RX(11)

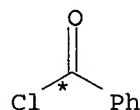
RX(63) A + B + 5 I + Z + 7 G + AL  
====> AM



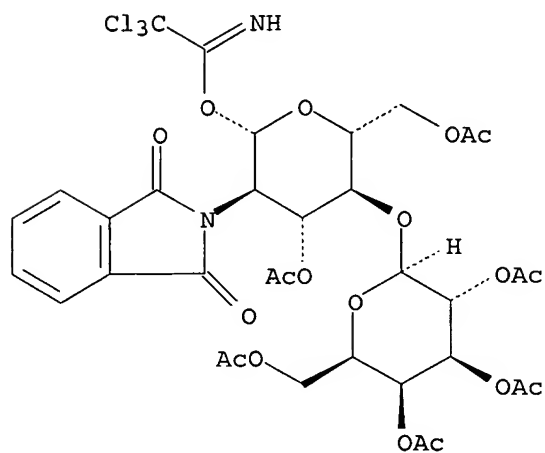
A



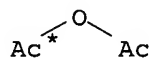
B



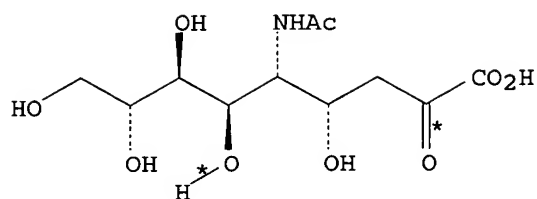
5 I



Z



7 G



AL

6  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(1) RCT A 63-42-3

STAGE(1)

RGT D 127-09-3 AcONa  
SOL 108-24-7 Ac2O

STAGE(2)

RCT B 108-98-5  
RGT E 109-63-7 BF3-Et2O

STAGE(3)

RGT F 124-41-4 NaOMe  
SOL 67-56-1 MeOH

PRO C 5329-58-8

RX(2) RCT C 5329-58-8

STAGE(1)

RGT K 3144-16-9 10-CSA, L 463-82-1 Propane, 2,2-dimethyl-, M  
121-44-8 Et3N  
SOL 67-56-1 MeOH, 7732-18-5 Water

STAGE(2)

RCT I 98-88-4  
SOL 110-86-1 Pyridine

STAGE(3)

RGT N 7647-01-0 HCl  
SOL 64-19-7 AcOH, 109-99-9 THF

PRO J 301662-92-0

RX(5) RCT J 301662-92-0, Z 87190-71-4

STAGE(1)

RGT E 109-63-7 BF3-Et2O  
SOL 75-09-2 CH2Cl2

STAGE(2)

RGT M 121-44-8 Et3N

PRO AA 301663-16-1



RX(9) RCT AA 301663-16-1

STAGE(1)

RGT F 124-41-4 NaOMe  
SOL 67-56-1 MeOH

STAGE(2)

RGT AC 302-01-2 N2H4

STAGE(3)

SOL 64-17-5 EtOH

STAGE(4)

RCT G 108-24-7  
SOL 110-86-1 Pyridine

STAGE(5)

SOL 67-56-1 MeOH

PRO AK 301663-18-3

RX(10) RCT AK 301663-18-3  
RGT F 124-41-4 NaOMe  
PRO AG 301663-21-8  
SOL 67-56-1 MeOH

RX(11) RCT AG 301663-21-8, AL 131-48-6

STAGE(1)

RGT AN 1310-73-2 NaOH, AO 65-47-4 Cytidine 5'-(tetrahydrogen triphosphate)

STAGE(2)

RGT AP 7786-30-3 MgCl2, AQ 3483-12-3 Cleland's reagent  
CAT 37237-43-7 Galactosyltransferase, uridine diphosphogalactose-glycoprotein, 148093-35-0 Cytidyltransferase, cytidine monophosphate-deoxynonulosonate

PRO AM 301663-35-4

NTE ENZYMADEC REACTION

AN 133:310068 CASREACT

TI Polymer-supported and chemoenzymatic synthesis of the Neisseria meningitidis pentasaccharide: a methodological comparison

AU Yan, Fengyang; Wakarchuk, Warren W.; Gilbert, Michel; Richards, James C.; Whitfield, Dennis M.

CS Institute for Biological Sciences, National Research Council of Canada, Ottawa, ON, K1A 0R6, Can.

SO Carbohydrate Research (2000), 328(1), 3-16  
CODEN: CRBRAT; ISSN: 0008-6215

PB Elsevier Science Ltd.

DT Journal

LA English

AB Neisseria meningitidis trisaccharide [GlcNAc $\beta$ (1 $\rightarrow$ 3)Gal $\beta$ (1.fwdarw.4)Glc-R], tetrasaccharide [Gal $\beta$ (1 $\rightarrow$ 4)GlcNAc $\beta$ (1.fwdarw.3)Gal $\beta$ (1 $\rightarrow$ 4)Glc-R], and a pentasaccharide [Neu5Ac $\alpha$ (2 $\rightarrow$ 3)Gal $\beta$ (1 $\rightarrow$ 4)GlcNAc $\beta$ (1 $\rightarrow$ 3)Gal $\beta$ (1 $\rightarrow$ 4)Glc-SPh] were prepared via conventional chemical synthesis, polymer-supported synthesis, and chemoenzymic methods, starting from

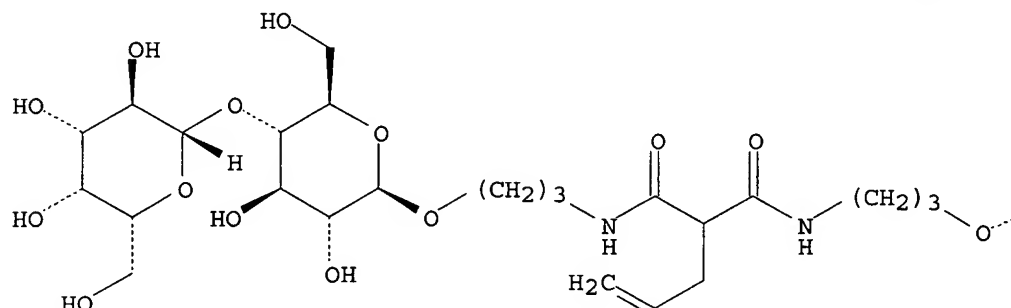
D-lactose. The polymer polyethyleneglycol monomethyl-ether (MPEG) and the linker dioxymethylene (DOX) were used with a lactose-bound acceptor to improve the purification process. Several enzymes (LgtA, GalE-LgtB fusion, and CMP-Neu5Ac synthetase/sialyltransferase fusion) were used for syntheses of these oligosaccharides. Excellent stereo- and regioselectivities as well as high yield (>90% from Gal $\beta$ (1 $\rightarrow$ 4)Glc-SPh) of the pentasaccharide were obtained. Both of the convenient processes are suitable for efficient preparation of target oligosaccharides.

RE.CNT 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

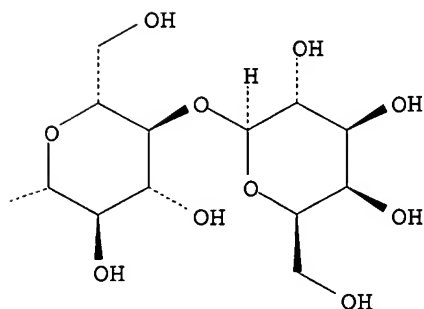
L6 ANSWER 26 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(13) OF 18 COMPOSED OF RX(5), RX(6)  
RX(13) 2 L + 3 F ==> U

PAGE 1-A

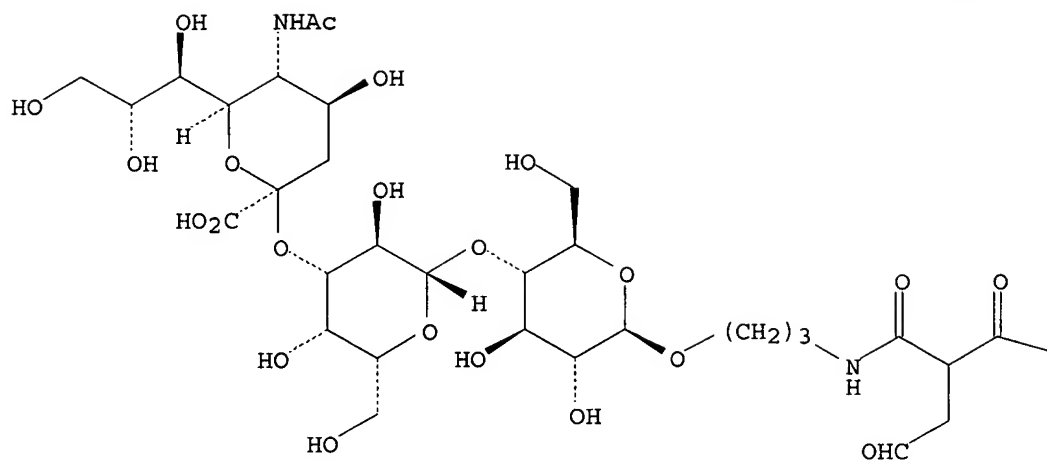


PAGE 1-B



L





\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(5) RCT L 273937-98-7, F 131-48-6  
 RGT H 7786-30-3 MgCl<sub>2</sub>, I 65-47-4 Cytidine  
 5'-(tetrahydrogen triphosphate)  
 PRO S 273937-99-8, T 273938-00-4  
 CAT 9067-82-7 Cytidyltransferase, acylneuraminate  
 SOL 7732-18-5 Water

RX(6) RCT S 273937-99-8  
 RGT V 10028-15-6 Ozone  
 PRO U 273938-01-5  
 SOL 67-56-1 MeOH

AN 133:43736 CASREACT

TI Allylmalonamide as a bivalent linker: synthesis of biantennary  
 GM3-saccharide-Keyhole limpet hemocyanin glycoconjugate and the immune  
 response in mice

AU Zou, Wei; Abraham, Mary; Gilbert, Michel; Wakarchuk, Warren W.; Jennings,  
 Harold J.

CS Institute for Biological Sciences, National Research Council of Canada,  
 Ottawa, ON, K1A 0R6, Can.

SO Glycoconjugate Journal (2000), Volume Date 1999, 16(9), 507-515  
 CODEN: GLJOEW; ISSN: 0282-0080

PB Kluwer Academic Publishers

DT Journal

LA English

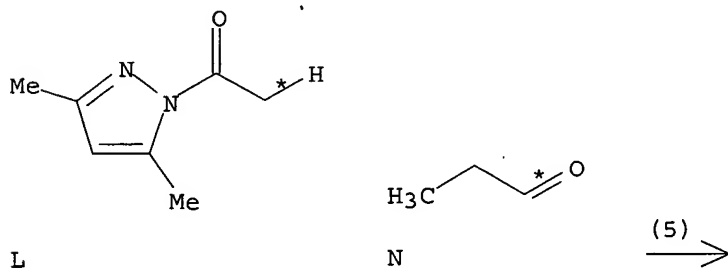
AB A biantennary GM3-saccharide (sialyllactoside) derivative was constructed  
 using allylmalonic acid as a bivalent linker, both carboxylic acids of  
 which were condensed with 3-aminopropyl lactoside prior to enzymic  
 sialylation with a fusion enzyme. The average ratios of saccharide to protein  
 were observed to be 35 in KLH conjugate and 9-12 in HSA conjugates. The  
 antisera obtained by immunizing mice with the biantennary  
 sialyllactoside-KLH conjugate together with MPL adjuvant were analyzed by  
 ELISA. Using several structurally related saccharide-HSA conjugates as  
 screening antigens, it was concluded that anti-sialyllactoside antibodies,  
 both IgG and IgM, were effectively raised. This was further supported by  
 competitive inhibition expts. using lactoside, sialyllactoside and

biantennary sialyllactoside as inhibitors.

RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 27 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(5) OF 31 L + N ==> O



O  
YIELD 51%

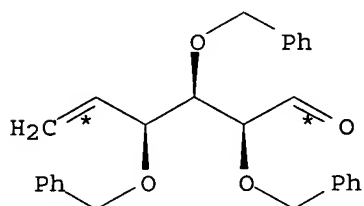
RX(5) RCT L 10199-63-0, N 123-38-6  
RGT I 29858-07-9 MgBr<sub>2</sub>-Et<sub>2</sub>O, J 7087-68-5 EtN(Pr-i)<sub>2</sub>  
PRO O 205592-92-3  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
AN 128:270563 CASREACT  
TI Stereocontrolled aldol reaction of N-acylpyrazoles with aldehydes using  
LDA or MgBr<sub>2</sub>-DIEA  
AU Kashima, Choji; Fukuchi, Iwao; Takahashi, Katsumi; Fukusaka, Kiyoshi;  
Hosomi, Akira  
CS Dep. Chem., Univ. Tsukuba, Ibaraki, 305, Japan  
SO Heterocycles (1998), 47(1), 357-365  
CODEN: HTCYAM; ISSN: 0385-5414  
PB Japan Institute of Heterocyclic Chemistry  
DT Journal  
LA English  
AB The aldol reaction of 1-acyl-3,5-dimethylpyrazoles via lithium enolate  
intermediates generated using LDA was kinetically controlled with syn  
stereoselectivity. On the other hand, the reaction carried out with DIEA  
in the presence of MgBr<sub>2</sub> under thermodyn. control proceeded with anti  
stereoselectivity. In the aldol reaction using 3-phenyl-1-menthopyrazole  
as a chiral auxiliary, the diastereoselectivity was ≤ 81% with  
predominant 2'S configuration.

RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

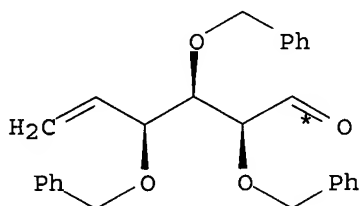
L6 ANSWER 28 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(15) OF 21 COMPOSED OF RX(3), RX(4), RX(5)

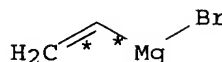
RX(15) 2 E + 2 I + 2 M ==> Q



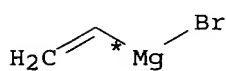
E



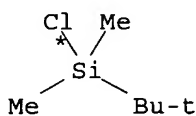
E



I

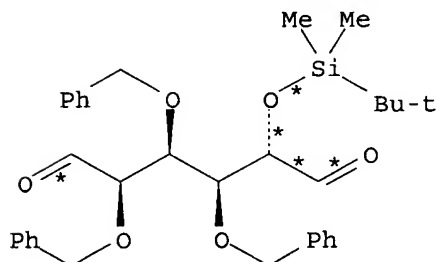


I



2 M

3  
STEPS  
→



Q

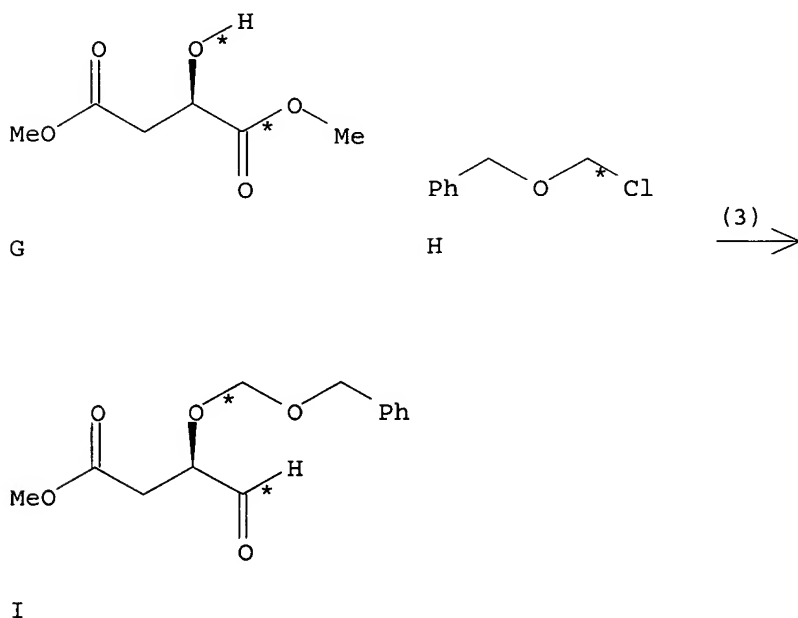
RX(3) RCT E 195873-65-5, I 1826-67-1  
RGT L 29858-07-9 MgBr2-Et2O  
PRO J 195873-66-6, K 195873-73-5  
SOL 75-09-2 CH2Cl2

RX(4) RCT J 195873-66-6, K 195873-73-5, M 18162-48-6  
RGT O 288-32-4 1H-Imidazole  
PRO N 195873-67-7  
SOL 68-12-2 DMF

RX(5) RCT N 195873-67-7  
RGT R 10028-15-6 Ozone, S 75-18-3 Me2S  
PRO Q 195873-68-8

SOL 110-86-1 Pyridine, 67-56-1 MeOH  
 AN 127:248323 CASREACT  
 TI Enantiospecific synthesis of a differentially protected L-chiro-inositol from D-xylose  
 AU Kornienko, Alexander; D'alarcao, Marc  
 CS Department of Chemistry, Tufts University, Medford, MA, 02155, USA  
 SO Tetrahedron Letters (1997), 38(37), 6497-6500  
 CODEN: TELEAY; ISSN: 0040-4039  
 PB Elsevier  
 DT Journal  
 LA English  
 AB A convenient synthesis of differentially protected L-chiro-inositol from 2,3,4-tri-O-benzyl-D-xylopyranose is described. The structure of the product was confirmed by its transformation to the pentabenzylated derivative of (-)-quebrachitol.  
 RE.CNT 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT  
 L6 ANSWER 29 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(3) OF 15 G + H ==> I...



RX(3) RCT G 70681-41-3, H 3587-60-8  
 STAGE(1)  
 RGT J 7087-68-5 EtN(Pr-i)2  
 SOL 75-09-2 CH2Cl2  
 STAGE(2)  
 RGT K 7789-48-2 MgBr2  
 SOL 75-09-2 CH2Cl2  
 STAGE(3)  
 RGT L 1191-15-7 AlH(Bu-i)2

SOL 110-54-3 Hexane

STAGE(4)

RGT M 67-56-1 MeOH

PRO I 175411-30-0

NTE (84%/66%)

AN 124:289063 CASREACT

TI A Direct Asymmetric Synthesis of Juglomycin A

AU Maeda, Hiroshi; Kraus, George A.

CS Department of Chemistry, Iowa State University, Ames, IA, 50011, USA

SO Journal of Organic Chemistry (1996), 61(9), 2986-7

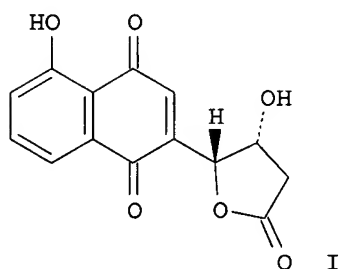
CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

LA English

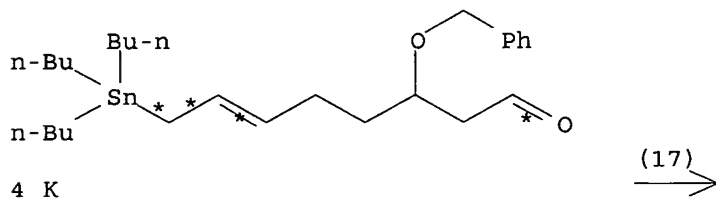
GI



AB Juglomycin A (I) has been synthesized in four steps from 5-methoxy-1-naphthol.

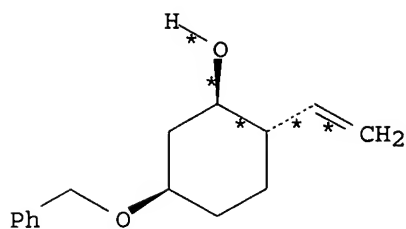
L6 ANSWER 30 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(17) OF 329 ...4 K ==> BC + BD + BE + BF...

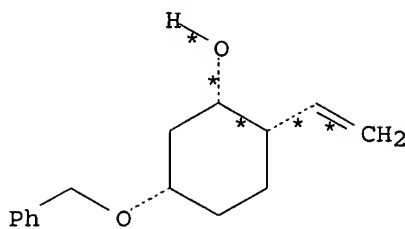


4 K

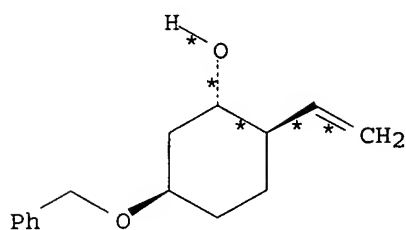




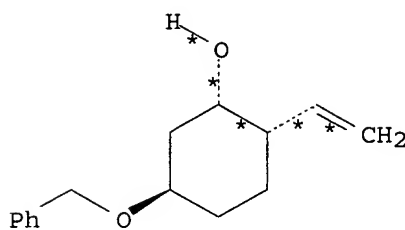
BC  
YIELD 93%(59)



BD  
YIELD 93%(30)



BE  
YIELD 97%(12)



BF  
YIELD 93%(4)

RX(17) RCT K 168208-39-7

STAGE(1)

RGT BG 29858-07-9 MgBr2-Et2O

SOL 75-09-2 CH2Cl2

STAGE(2)

RGT AZ 144-55-8 NaHCO3

PRO BC 155433-91-3, BD 168208-54-6, BE 155433-92-4, BF 155433-95-7

NTE stereoselective, optimized on agent, alternative preparation shown

AN 123:227660 CASREACT

TI Intramolecular Allylstannane-Aldehyde Cyclizations: Stereochemical Results with Flexible Tethers for Reactions Forming Vinylcyclohexanols

AU Keck, Gary E.; Dougherty, Shawn M.; Savin, Kenneth A.

CS Department of Chemistry, University of Utah, Salt Lake City, UT, 84112, USA

SO Journal of the American Chemical Society (1995), 117(23), 6210-23

CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

DT Journal

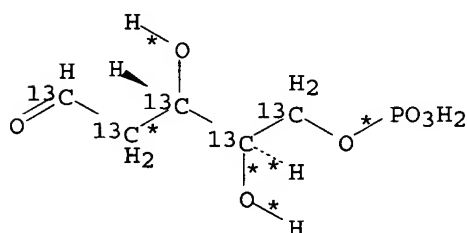
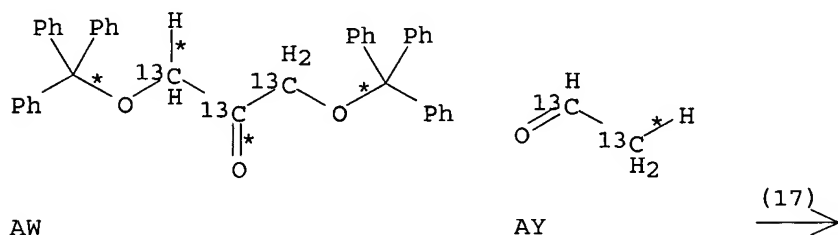
LA English

AB Intramol. Lewis acid-promoted cyclization reactions of both (Z)- and (E)-3-phenyl-8-(tri-n-butylstannyl)oct-6-enal and (Z)- and (E)-3-(benzyloxy)-8-(tri-n-butylstannyl)oct-6-enal have been examined using a variety of Lewis acids, specifically BF3.Et2O, CF3CO2H, SnCl4, TiCl4, and MgBr2.Et2O. Thermally promoted cyclizations were also examined. The results show that product stereochem. is a sensitive function of both olefin stereochem. and Lewis acid. The data acquired in these studies

also suggest that such reactions are mechanistically more complex than previous studies with more constrained systems have revealed.

L6 ANSWER 31 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(17) OF 30 ...AW + AY ==> AZ



AZ  
YIELD 79%

RX(17) RCT AW 163928-33-4

STAGE(1)

CAT 6192-52-5 p-MeC6H4SO3H.H2O  
SOL 67-56-1 MeOH, 75-09-2 CH2Cl2  
CON 17 hours, room temperature

STAGE(2)

RGT X 1310-73-2 NaOH  
SOL 7732-18-5 Water  
CON room temperature, neutralized

STAGE(3)

RCT AY 1632-98-0  
RGT BA 5541-93-5 2-Propenoic acid, 2-(phosphonoxy)-, trisodium salt, BB 56-65-5 Adenosine 5'-(tetrahydrogen triphosphate), BC 7786-30-3 MgCl2, BD 7447-40-7 KCl  
CAT 9026-97-5 Aldolase, deoxyribo-, 9030-66-4 Kinase (phosphorylating), glycerol, 9001-59-6 Kinase (phosphorylating), pyruvate, 9023-78-3 Isomerase, triose phosphate  
SOL 7732-18-5 Water  
CON 49 hours, room temperature, pH 7.4

STAGE(4)

RGT X 1310-73-2 NaOH

CON room temperature, pH 8

## STAGE(5)

RGT BE 10326-27-9 Barium chloride (BaCl<sub>2</sub>), dihydrate  
CON 40 minutes, room temperature

## STAGE(6)

RGT BF 12640-54-9 DOWEX 50  
SOL 7732-18-5 Water  
CON 3 hours, room temperature

## STAGE(7)

RGT X 1310-73-2 NaOH  
SOL 7732-18-5 Water  
CON room temperature, pH 7

PRO AZ 163928-35-6

NTE biotransformation, stereoselective, enzymic(third stage,  
recombinant 2-deoxyribose-5-phos 7786-30-3 MgCl<sub>2</sub>, BD  
7447-40-7 KCl9026-97-5 Aldolase, deoxyribo-, 9030-66-4 Kinase  
(phosphorylating), glycerol, 9001-59-6 Kinase (phosphorylating),  
pyruvate, 9023-78-3 Isomerase, triose phosphate7732-18-5 Water

AN 123:28423 CASREACT

TI Recombinant 2-Deoxyribose-5-phosphate Aldolase in Organic Synthesis: Use  
of Sequential Two-Substrate and Three-Substrate Aldol Reactions

AU Wong, Chi-Huey; Garcia-Junceda, Eduardo; Chen, Lihren; Blanco, Olga;  
Gijzen, Harrie J. M.; Steensma, Darryl H.

CS Department of Chemistry, Scripps Research Institute, La Jolla, CA, 92037,  
USA

SO Journal of the American Chemical Society (1995), 117(12), 3333-9  
CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

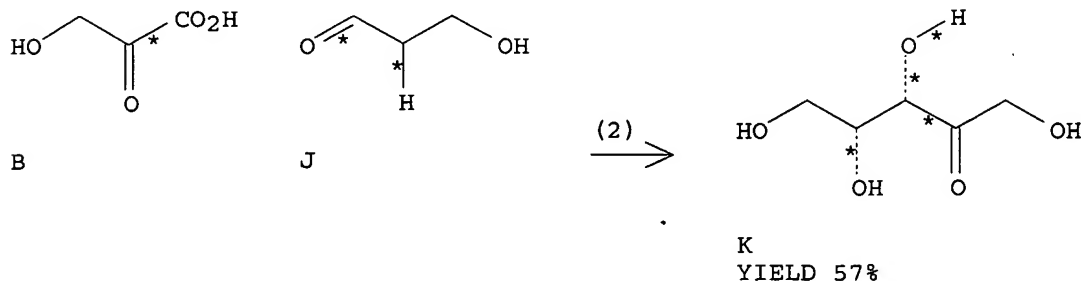
DT Journal

LA English

AB A new procedure has been developed for the large scale preparation of  
recombinant 2-deoxyribose-5-phosphate aldolase (DERA, EC 4.1.2.4) from E.  
coli strain DH5a (ATCC 86963). The enzyme was purified to homogeneity  
with an overall yield of 83% and in sufficient quantity to grow crystals  
suitable for x-ray diffraction studies. Using the sequential two- or  
three-substrate aldol reaction, DERA was applied to the synthesis of a  
variety of sugar analogs including deoxyriboses, 2-deoxyfucose analogs,  
dideoxyhexoses, trideoxyhexoses, deoxythiosugars, and <sup>13</sup>C-substituted  
2-deoxyribose-5-phosphate.

L6 ANSWER 32 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(2) OF 6 B + J ==> K



RX(2) RCT B 1113-60-6, J 2134-29-4

STAGE(1)

RGT D 7786-30-3 MgCl<sub>2</sub>, E 136-09-4 Thiazolium,  
3-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-4-methyl-5-  
(4,6,6-trihydroxy-4,6-dioxido-3,5-dioxa-4,6-diphosphahex-1-  
yl)-, inner salt, F 7647-01-0 HCl  
CAT 9014-48-6 Transketolase  
SOL 7732-18-5 Water

STAGE(2)

SOL 64-17-5 EtOH

PRO K 551-84-8

NTE biotransformation, enzymic, buffered soln., stereoselective, in  
the dark, spinach transketolase used

AN 120:245607 CASREACT

TI Study of the specificity of a spinach transketolase on achiral substrates

AU Dalmas, Valerie; Demuynck, Colette

CS Lab. Chim. Org. Biol., Univ. Blaise Pascal, Aubiere, 63177, Fr.

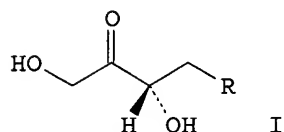
SO Tetrahedron: Asymmetry (1993), 4(11), 2383-8

CODEN: TASYE3; ISSN: 0957-4166

DT Journal

LA English

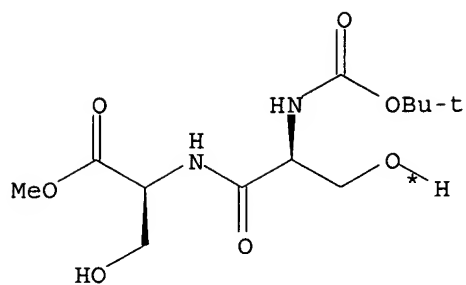
GI



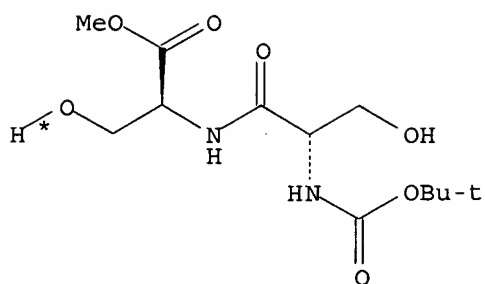
AB The behavior and the specificity of a spinach transketolase towards  
achiral aldehydes RCH<sub>2</sub>CHO (R = H, OH, OMe, SMe, CH<sub>2</sub>OH, CH<sub>2</sub>SMe) with  
hydroxypyruvate HOCH<sub>2</sub>C(O)CO<sub>2</sub>H was studied. The authors have shown that  
these aldehydes are accepted by the enzyme and yield the corresponding  
saccharides I with good enantiomeric excess.

L6 ANSWER 33 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

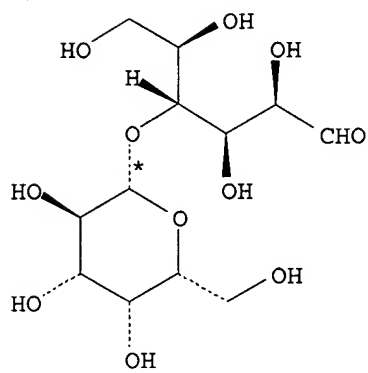
RX(2) OF 7 2 H + 2 B ==> I + J



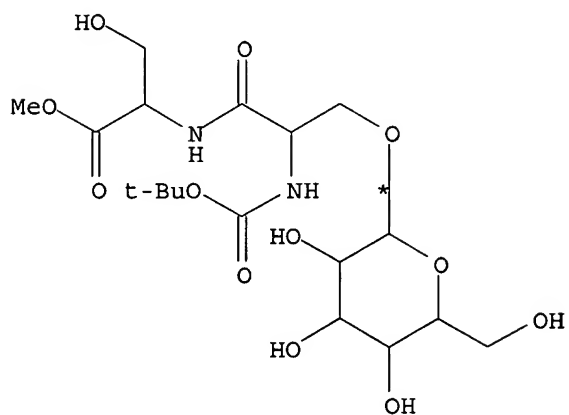
H



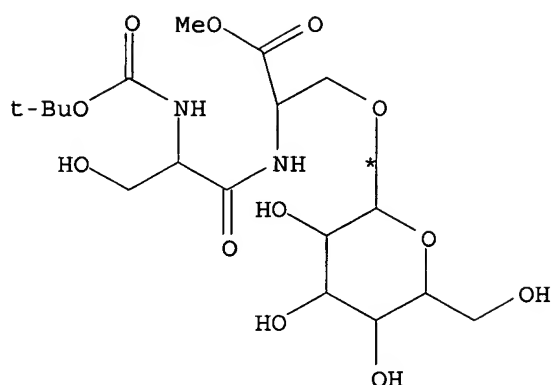
H



2 B



I



J

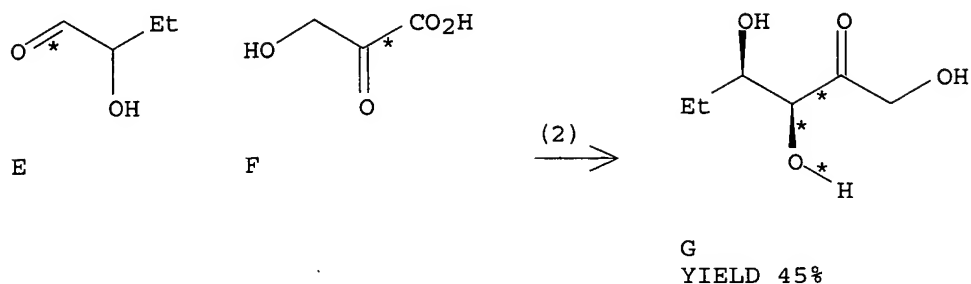
RX(2) RCT H 84728-07-4, B 63-42-3  
 RGT D 7786-30-3 MgCl<sub>2</sub>, E 3483-12-3 Cleland's reagent  
 PRO I 145520-98-5, J 145521-08-0  
 CAT 9031-11-2 Galactosidase,  $\beta$ -  
 SOL 7732-18-5 Water  
 NTE 11% overall / enzymic / buffered  
 AN 118:60111 CASREACT  
 TI Enzymic synthesis of  $\beta$ -galactosyl dipeptides and of  
 $\beta$ -1,3-digalactosylserine derivatives using  $\beta$ -galactosidase  
 AU Attal, Sandra; Bay, Sylvie; Cantacuzene, Daniele  
 CS Dep. Biochim. Genet. Mol., Inst. Pasteur, Paris, 75724, Fr.  
 SO Tetrahedron (1992), 48(42), 9251-60  
 CODEN: TETRAB; ISSN: 0040-4020  
 DT Journal  
 LA English  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

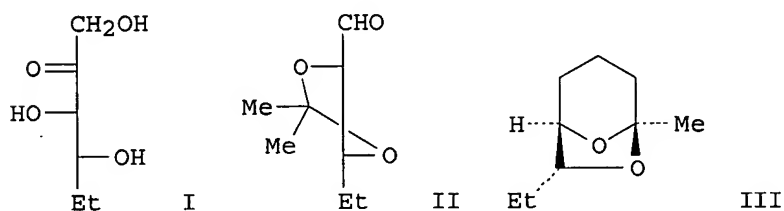
AB The transgalactosidation from lactose to dipeptides has been achieved using  $\beta$ -galactosidase from *Escherichia coli* as catalyst. Two series of dipeptides have been studied, each of them containing a serine residue. Thus, the  $\beta$ -galactosidase-catalyzed reaction of lactose with dipeptides R-Ser-X-OMe [I; R = Me<sub>3</sub>CO<sub>2</sub>C (Boc), allyloxycarbonyl (Aloc); X = Gly, Ala] gave  $\beta$ -galactosyl dipeptides II, whereas the  $\beta$ -galactosidase-catalyzed reaction of lactose with dipeptides R<sub>1</sub>-X<sub>1</sub>-Ser-OMe (R<sub>1</sub> = Boc, Aloc; X<sub>1</sub> = Gly, Ala), gave  $\beta$ -galactosyl dipeptides III. The  $\beta$ -galactosidase-catalyzed reaction of lactose with I (R = Boc, Aloc; X = Ser) gave a mixture of two regioisomers with O-galactosylation at each serine hydroxy group. The  $\beta$ -galactosidase-catalyzed reaction of serine galactoside IV with lactose gave a mixture of digalactosyl derivs. V and VI. The best condensations occur when serine is at the N-terminal end of the dipeptide. Mild hydrolysis of the ester group of the labile glycosyl dipeptide derivs. has been achieved using subtilisin. The condensation of lactose with  $\beta$ -galactosyl serine gave  $\beta$ -1,3-digalactoxyl-serine derivs.

L6 ANSWER 34 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(2) OF 15 E + F ==&gt; G...



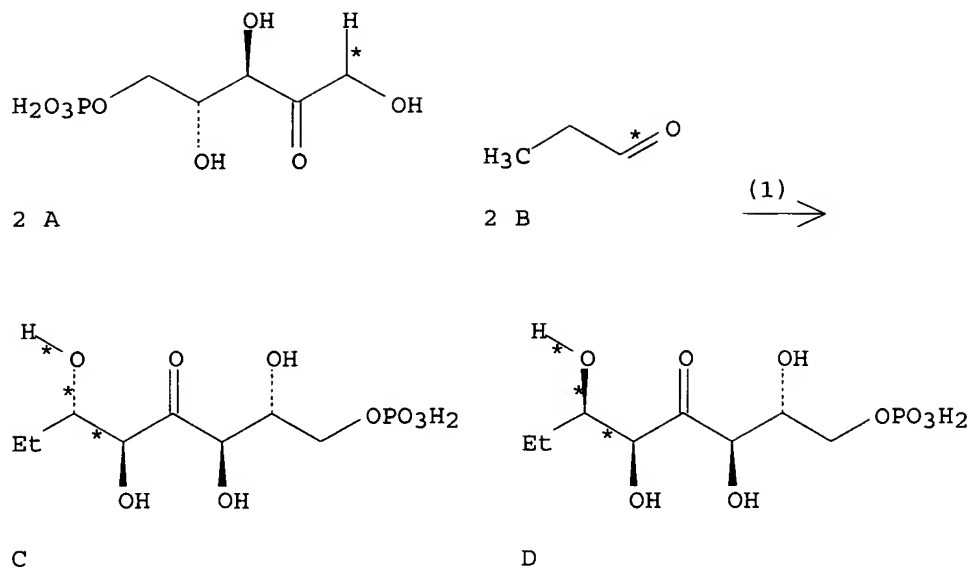
RX(2) RCT E 37428-67-4, F 1113-60-6  
 RGT H 7786-30-3 MgCl<sub>2</sub>, I 154-87-0 Thiazolium,  
 3-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-4-methyl-5-(4,6,6-trihydroxy-4,6-dioxido-3,5-dioxo-4,6-diphosphahex-1-yl)-, chloride, J 9014-48-6 Transketolase  
 PRO G 117625-98-6  
 AN 115:280403 CASREACT  
 TI A transketolase-based synthesis of (+)-exo-brevicomine  
 AU Myles, David C.; Andrulis, Peter J., III; Whitesides, George M.  
 CS Dep. Chem., Harvard Univ., Cambridge, MA, 02138, USA  
 SO Tetrahedron Letters (1991), 32(37), 4835-8  
 CODEN: TELEAY; ISSN: 0040-4039  
 DT Journal  
 LA English  
 GI



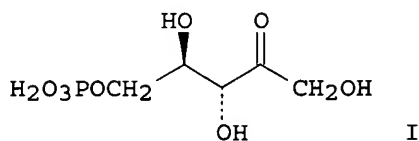
AB The com. available enzyme transketolase (EC 2.2.1.1) catalyzed the condensation of  $\beta$ -hydroxypyruvic acid and 2-hydroxybutyraldehyde to furnish the central intermediate in the sequence, optically active hydroketone I. A short sequence converted I to protected aldose II. Wittig extension of the aldehyde followed by hydrogenation and ketal hydrolysis generated the naturally occurring beetle pheromone title compound (III).

L6 ANSWER 35 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(1) OF 1 2 A + 2 B ==&gt; C + D



RX(1)      RCT    A 551-85-9, B 123-38-6  
              RGT    E 7786-30-3 MgCl<sub>2</sub>  
              PRO    C 136083-09-5, D 136083-10-8  
              CAT    55576-36-8 Synthase, 3-hexulose phosphate  
              SOL    7732-18-5 Water  
              NTE    equil., stereoselective  
 AN    115:136506    CASREACT  
 TI    Enzyme-catalyzed aldol reactions with 3-hexulose phosphate synthase  
 AU    Beisswenger, Roswitha; Snatzke, Guenther; Thiem, Joachim; Kula, Maria Regina  
 CS    Inst. Enzymtechnol., Heinrich-Heine-Univ. Duesseldorf, Juelich, D-5170, Germany  
 SO    Tetrahedron Letters (1991), 32(27), 3159-62  
       CODEN: TELEAY; ISSN: 0040-4039  
 DT    Journal  
 LA    English  
 GI

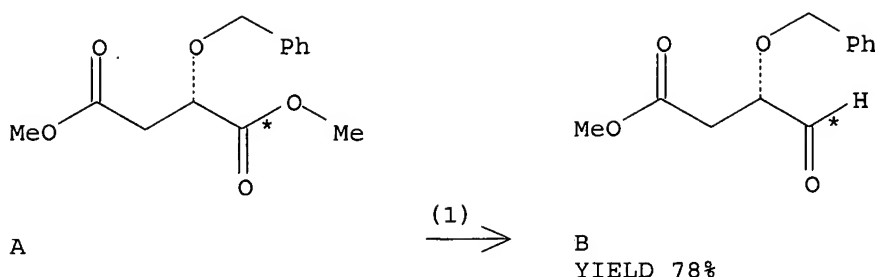


AB    3-Hexulose phosphate synthase catalyzes the aldol reactions between ribulose phosphate I and a rather wide range of aldehydes. The stereoselectivity of the reaction was investigated with propionaldehyde as substrate. The sense of chirality at C5 is definite, but 2 isomers at C6 are formed during formation of the new C-C bond.

L6    ANSWER 36 OF 41    CASREACT    COPYRIGHT 2005 ACS on STN

RX(1) OF 11      A ==> B...





RX(1) RCT A 82130-73-2  
 RGT C 1191-15-7 AlH(Bu-i)<sub>2</sub>, D 22873-23-0 Ethane,  
 1,1'-oxybis-, compd. with magnesium bromide (MgBr)  
 PRO B 129151-77-5  
 SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>, 108-88-3 PhMe  
 AN 114:42022 CASREACT  
 TI A useful new enantiomerically pure synthon from malic acid: chelation  
 controlled activation as a route to regioselectivity  
 AU Keck, Gary E.; Andrus, Merritt B.; Romer, Duane R.  
 CS Dep. Chem., Univ. Utah, Salt Lake City, UT, 84112, USA  
 SO Journal of Organic Chemistry (1991), 56(1), 417-20  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DT Journal  
 LA English  
 AB The effect of chelation in allowing regioselective ester redns. has been  
 examined Reduction of the malic acid derivative (S)-MeO<sub>2</sub>CCH<sub>2</sub>CH(OCH<sub>2</sub>Ph)CO<sub>2</sub>H  
 with diisobutylaluminum hydride in the presence of stoichiometric amts. of  
 magnesium bromide-etherate cleanly affords aldehyde (S)-  
 MeO<sub>2</sub>CCH<sub>2</sub>CH(OCH<sub>2</sub>Ph)CHO (I); in the absence of magnesium bromide, mixts. of  
 all possible reduction products are produced. The same procedure has been  
 successfully applied to diester (S)-MeO<sub>2</sub>CCH<sub>2</sub>CH<sub>2</sub>CH(OCH<sub>2</sub>OCH<sub>2</sub>Ph)CO<sub>2</sub>Me.  
 Further stereoselective elaborations of I are described.

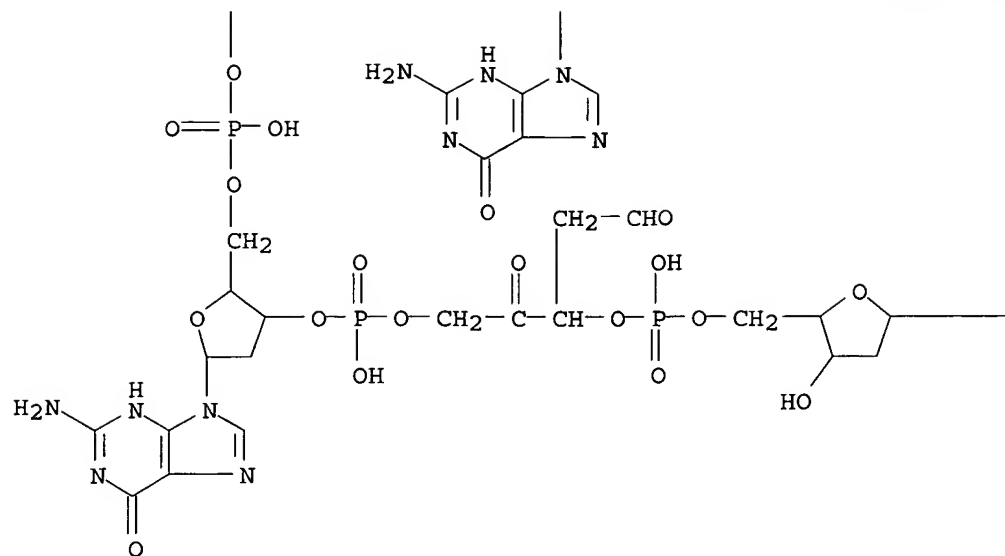
L6 ANSWER 37 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(33) OF 49 COMPOSED OF RX(2), RX(3), RX(4)

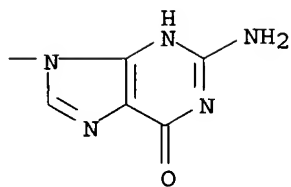
RX(33) 3 B ==> Q + R

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

PAGE 2-A



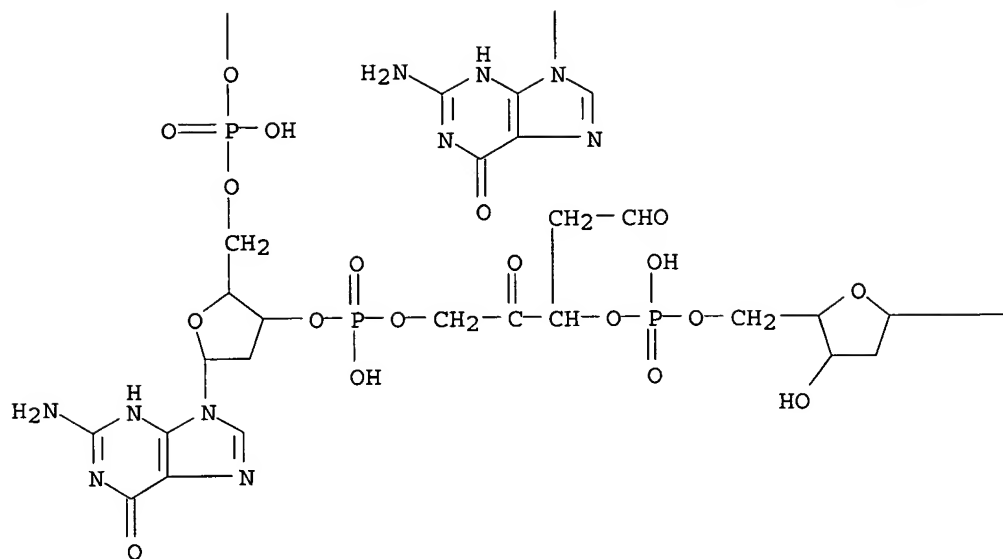
PAGE 2-B



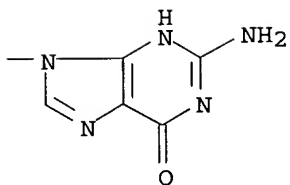
B

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

PAGE 2-A



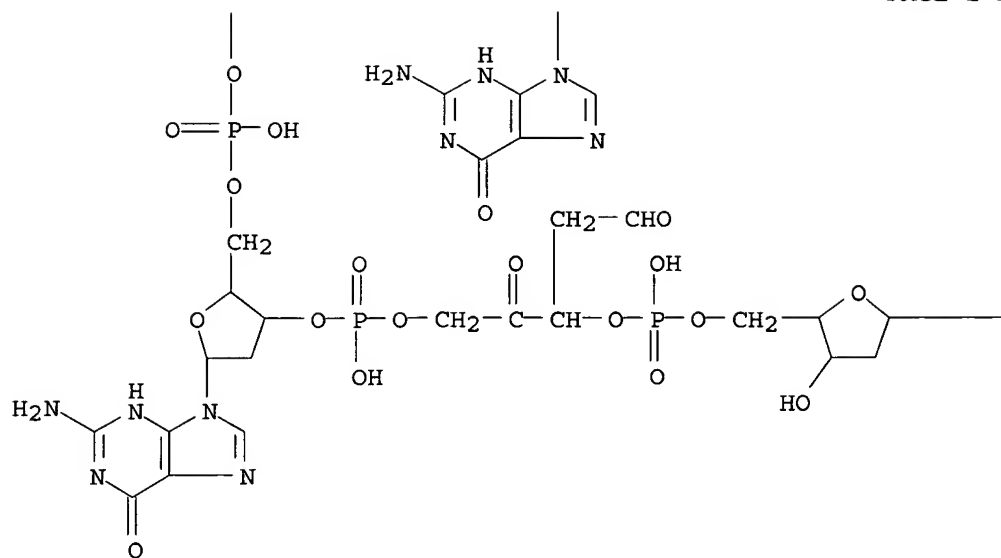
PAGE 2-B



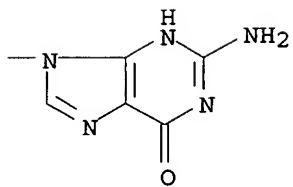
B

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

PAGE 2-A

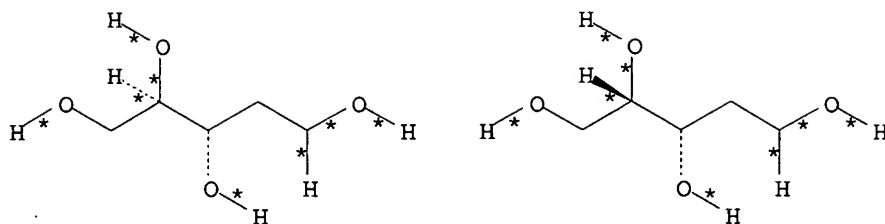


PAGE 2-B



B

3  
STEPS  
→



Q

R

RX(2) RCT B 126502-68-9  
 RGT J 16940-66-2 NaBH4  
 PRO H 126502-69-0, I 127001-06-3  
 SOL 7365-45-9 HEPES  
 NTE 92% overall

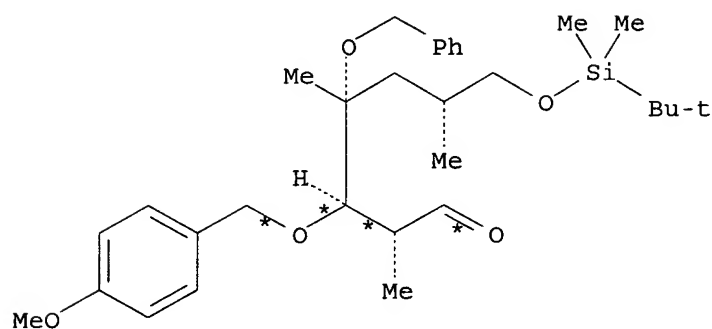
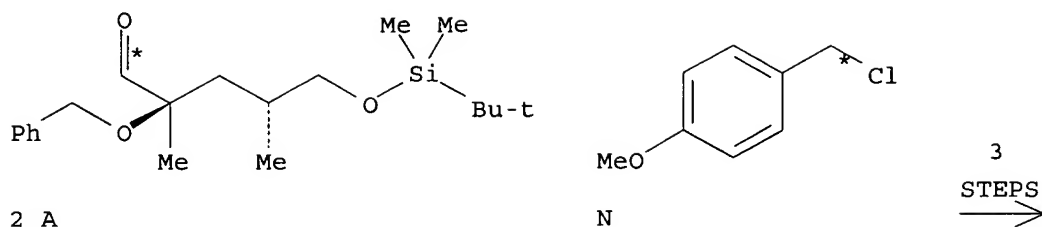
RX(3) RCT H 126502-69-0, I 127001-06-3  
 RGT M 127-09-3 AcONa, N 7646-85-7 ZnCl2, O 54576-84-0 Nuclease,  
 Penicillium citrinum, P1  
 PRO K 104779-62-6, L 104870-73-7  
 SOL 7732-18-5 Water

RX(4) RCT K 104779-62-6  
 RGT S 7786-30-3 MgCl2, T 9025-82-5 Phosphodiesterase  
 PRO Q 13942-76-2, R 104870-74-8

AN 113:115745 CASREACT  
 TI Identification and quantitation of the lesion accompanying base release in  
 bleomycin-mediated DNA degradation  
 AU Rabow, Lois E.; Stubbe, JoAnne; Kozarich, John W.  
 CS Coll. Agric. Life Sci., Univ. Wisconsin, Madison, WI, 53706, USA  
 SO Journal of the American Chemical Society (1990), 112(8), 3196-203  
 CODEN: JACSAT; ISSN: 0002-7863  
 DT Journal  
 LA English  
 AB Interaction of bleomycin, Fe2+, and limiting O or bleomycin, Fe+3, and  
 H2O2 with DNA results in the production of free nucleic acid base and an  
 oxidatively damaged sugar lesion that undergoes strand scission subsequent  
 to treatment with alkali. The hexamer d(CGCGCG) was utilized to develop a  
 protocol to establish the identity of this lesion as a  
 2'-deoxy-4'-pentulose moiety and to establish its stoichiometric production  
 with respect to free nucleic acid base. The protocol developed was  
 extended to a variety of heterogeneous DNAs with similar results. The  
 predominant pathway for base release in bleomycin-mediated DNA degradation is  
 the result of chemical at C(4') of the sugar moiety.

L6 ANSWER 38 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(33) OF 55 COMPOSED OF RX(1), RX(4), RX(12)  
 RX(33) 2 A + N ==> AH



AH  
YIELD 73%

RX(1) RCT A 114114-18-0  
RGT D 7789-48-2 MgBr<sub>2</sub>, E 31197-41-8 Stannane,  
2-butenyltributyl-  
PRO B 114114-19-1, C 114181-54-3  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

RX(4) RCT B 114114-19-1, N 824-94-2  
RGT P 7646-69-7 NaH  
PRO O 123493-56-1  
SOL 68-12-2 DMF

RX(12) RCT O 123493-56-1  
RGT AB 10028-15-6 Ozone  
PRO AH 114114-20-4  
CAT 110-86-1 Pyridine  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

AN 111:214284 CASREACT

TI Synthesis of macrolide antibiotics. 17. Synthesis of the A and B  
erythronolides (C1-C10) segments

AU Sviridov, A. F.; Borodkin, V. S.; Ermolenko, M. S.; Yashunskii, D. V.

CS Inst. Org. Khim. im. Zelinskogo, Moscow, USSR

SO Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1989), (3), 680-7  
CODEN: IASKA6; ISSN: 0002-3353

DT Journal

LA Russian

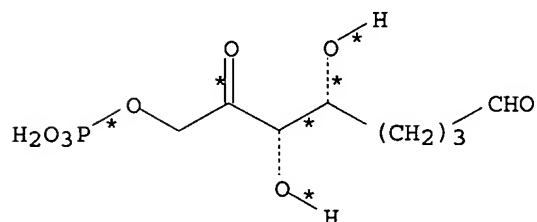
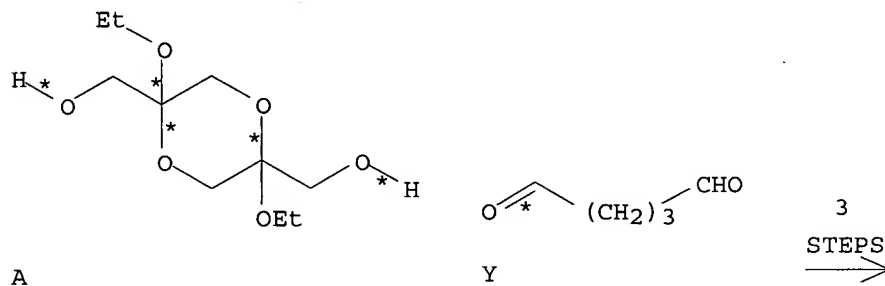
GI

L6 ANSWER 39 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

```

RX(35) OF 54 COMPOSED OF RX(1), RX(2), RX(8)
RX(35)      A  +  Y  ==>  Z

```



RX (1) RCT A 18294-29-6

RGT C 10025-87-3 POCl3  
SOL 110-86-1 Pyridine

RGT D 144-55-8 NaHCO<sub>3</sub>, E 1310-73-2 NaOH  
SOL 7732-18-5 Water

RGT F 7786-30-3 MgCl<sub>2</sub>, G 12125-02-9 NH<sub>4</sub>Cl

STAGE (4)

RGT H 10361-37-2 BaCl<sub>2</sub>  
SOL 64-17-5 EtOH

PRO B 113125-24-9

RX (2) RCT B 113125-24-9  
RGT M 61642-53-3 Dowex 50WX  
PRO L 57-04-5  
SOL 7732-18-5 Water

RX (8) RCT L 57-04-5, Y 111-30-8  
RGT P 9024-52-6 Fructoaldolase  
PRO Z 113125-29-4  
SOL 7732-18-5 Water

AN 108:112564 CASREACT

TI A novel convenient preparation of dihydroxyacetone phosphate and its use in enzymatic aldol reactions

AU Effenberger, Franz; Straub, Alexander

CS Inst. Org. Chem., Univ. Stuttgart, Stuttgart, D-7000/80, Fed. Rep. Ger.

SO Tetrahedron Letters (1987), 28(15), 1641-4

CODEN: TELEAY; ISSN: 0040-4039

DT Journal

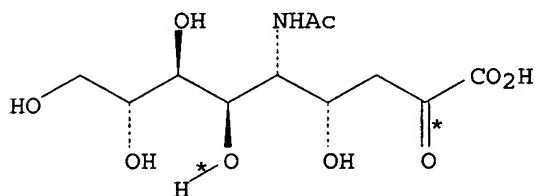
LA English

AB A new preparation of the stable barium salt of 2,5-bis(phosphonooxymethyl)-2,5-diethoxy-1,4-dioxane is described, which by treatment with DOWEX 50 H<sup>+</sup> gives dihydroxyacetone phosphate (DHAP) in high yield. DHAP prepared by this method was used for aldolase-catalyzed condensations.

L6 ANSWER 40 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

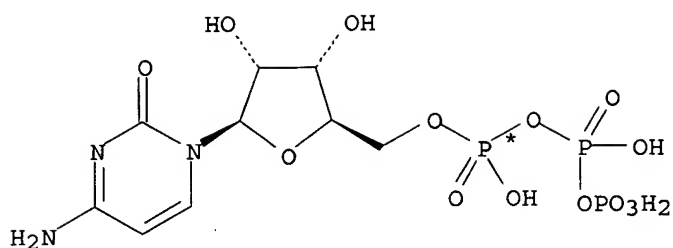
RX (5) OF 6 COMPOSED OF RX (2), RX (3)

RX (5) E + F + C ==> I

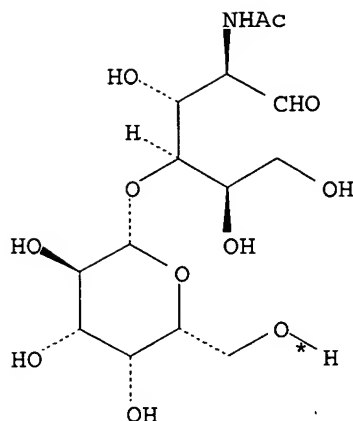


E





F



C

2

STEPS



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

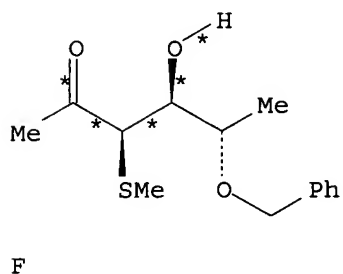
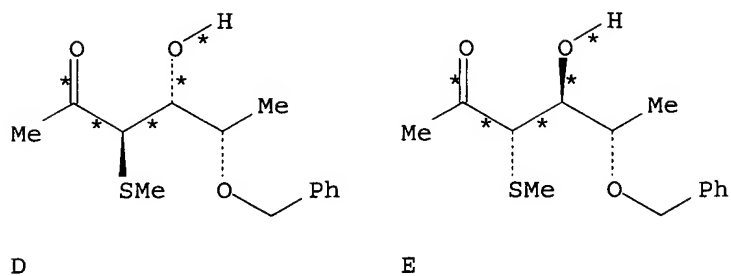
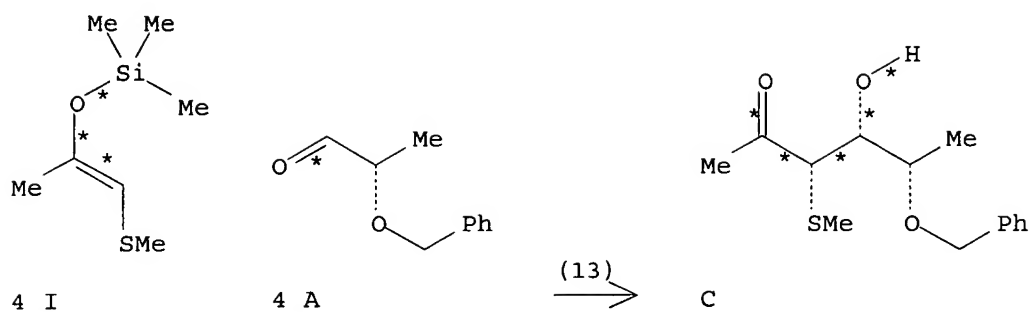
RX(2) RCT E 131-48-6, F 65-47-4  
 RGT H 9067-82-7D Cytidylyltransferase, acylneuraminate  
 PRO G 3063-71-6

RX(3) RCT C 32181-59-2, G 3063-71-6  
 RGT J 9075-81-4D Sialyltransferase, cytidine  
 monophosphoacetylneuraminate-galactosylglycoprotein, K  
 7786-30-3 MgCl<sub>2</sub>  
 PRO I 78969-47-8  
 NTE albumin

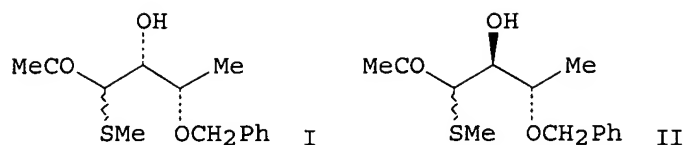
AN 106:33411 CASREACT  
 TI Synthesis of the trisaccharide Neu-5-Ac- $\alpha$ (2  $\rightarrow$  6)Gal- $\beta$ (1  
 $\rightarrow$  4)GlcNAc with immobilized enzymes  
 AU Thiem, Joachim; Treder, Wolfgang  
 CS Org. Chem. Inst., Univ. Muenster, Muenster, D-4400, Fed. Rep. Ger.  
 SO Angewandte Chemie (1986), 98(12), 1100-1  
 CODEN: ANCEAD; ISSN: 0044-8249  
 DT Journal  
 LA German  
 AB The title compound was prepared in 52% yield by coupling N-acetylactosamine  
 with cytidine 5'-monophosphosialate, using polymer-bound  
 $\beta$ -D-galactoside-(2 $\rightarrow$ 6)-sialyltransferase (E.C. 2.4.99.1). The  
 starting materials were also prepared with polymer-bound enzymes.

L6 ANSWER 41 OF 41 CASREACT COPYRIGHT 2005 ACS on STN

RX(13) OF 31 4 I + 4 A ==> C + D + E + F



RX(13)      RCT    I 99315-48-7, A 81445-44-5  
               RGT    Q 7789-48-2 MgBr<sub>2</sub>  
               PRO    C 102919-65-3, D 102919-66-4, E 102919-67-5, F  
                          103000-75-5  
               SOL    75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
 AN    105:42308    CASREACT  
 TI    Lewis acid mediated 1,2-asymmetric lk-induction to α-alkoxyaldehyde:  
       synthesis of α-nonsubstituted β,γ-syn-dihydroxy ketone  
       and ester  
 AU    Uenishi, Junichi; Tomozane, Hideo; Yamato, Masatoshi  
 CS    Fac. Pharm. Sci., Okayama Univ., Okayama, 700, Japan  
 SO    Tetrahedron Letters (1985), 26(29), 3467-70  
       CODEN: TELEAY; ISSN: 0040-4039  
 DT    Journal  
 LA    English  
 GI



AB Treatment of (S)-PhCH<sub>2</sub>OCHMeCHO with MeSCH:CMeOSiMe<sub>3</sub> and MgBr<sub>2</sub> in CH<sub>2</sub>Cl<sub>2</sub> gave 70% benzyloxyhydroxy ketones I and II in the ratio of 99:1. Other Lewis acids (SnCl<sub>4</sub>, ZnCl<sub>2</sub>, ZnI<sub>2</sub>, ZrCl<sub>4</sub>, FeCl<sub>3</sub>) also gave I as the major product. II was the major product when SnBr<sub>2</sub>, BF<sub>3</sub>·OEt<sub>2</sub>, and ZnCl<sub>2</sub>-THF were used.

=> dis his

(FILE 'HOME' ENTERED AT 16:08:17 ON 13 DEC 2005)

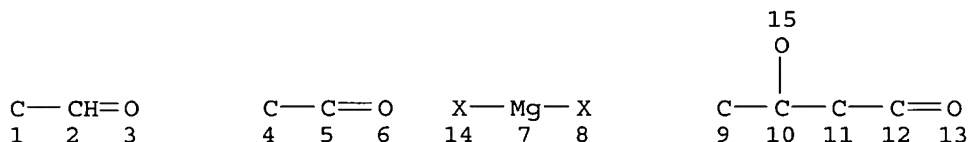
FILE 'REGISTRY' ENTERED AT 16:08:21 ON 13 DEC 2005

FILE 'CASREACT' ENTERED AT 16:08:24 ON 13 DEC 2005

L1 STR  
L2 6 S L1  
L3 118 S L1 FUL  
L4 STR  
L5 77 SEARCH L4 SUB=L3 FUL  
L6 41 S L3 NOT L5

=> d l6 que stat

L1 STR



NODE ATTRIBUTES:  
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE  
L3 118 SEA FILE=CASREACT SSS FUL L1 ( 1302 REACTIONS)  
L4 STR  
Li 1

NODE ATTRIBUTES:  
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

NUMBER OF NODES IS 1

STEREO ATTRIBUTES: NONE

L5 77 SEA FILE=CASREACT SUB=L3 SSS FUL L4 ( 1060 REACTIONS)  
L6 41 SEA FILE=CASREACT ABB=ON PLU=ON L3 NOT L5

=> log y

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
311.97	312.61

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-27.88	-27.88

CA SUBSCRIBER PRICE

STN INTERNATIONAL LOGOFF AT 16:12:31 ON 13 DEC 2005

FOR OFFICIAL USE ONLY

173260

ACCESS DB #

PLEASE PRINT CLEARLY

Scientific and Technical Information Center

# SEARCH REQUEST FORM

Requester's Full Name: MARK BERCH Examiner #: 59193 Date: 12/2/05  
Art Unit: 1624 Phone Number: 2- 0663 Serial Number: 10/69331  
Location (Bldg/Room#): 5C01 (Mailbox #): 5C18 Results Format Preferred (circle): PAPER DISK  
\*\*\*\*\*

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:

Title of Invention: \_\_\_\_\_

Inventors (please provide full names): \_\_\_\_\_

Earliest Priority Date: \_\_\_\_\_

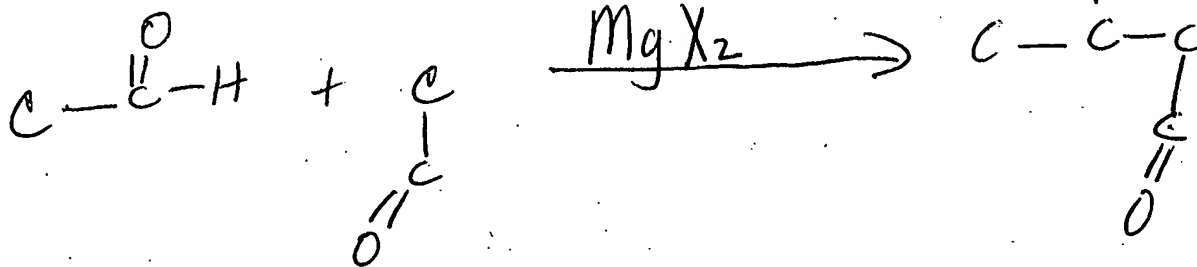
## Search Topic:

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

\*For Sequence Searches Only\* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

~~VOID~~

CAS react



X = Halogen

Exclude any reaction which uses a Li compound in this step

alternative to 6268393

1612  
1608

RECEIVED  
DEC - 2 2005  
ASR/RECH. DIVISION  
(STIC)

**THIS PAGE BLANK (USPTO)**